

Request - Jan Deval

Accession DB# 47188

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Sabirha Dey Examiner #: 74141 Date: 3/7/05
Art Unit: 1616 Phone Number: 20622 Serial Number: 09/508,934
Mail Box and Bldg/Room Location: 4C70, Rm, 4A45 Results Format Preferred (circle): PAPER DISK E-MAIL
if more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Andrew Steinmeyer et al
Inventors (please provide full names): New Vitamin D Derivatives

Earliest Priority Filing Date: 2/29/1998 PCT/EP98/06159

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Elected Group II Cls 1-3, 5, 6, 14, 20-28, 30-45.
R₁, R₂ form a methylene gp
V + W form a double bond.
R₃ + R₄ form H, alkyl.
V, I, D Compds, compositions and their process of making
See formula 1 in cl 1.

Please see attached sheet

Thank you

STAFF USE ONLY

	Type of Search	Vendors and cost where applicable
Searcher: <u>Jan</u>	NA Sequence #	STN <input checked="" type="checkbox"/>
Searcher: <u>22504</u>	AA Sequence #	Dialog
Searcher Location	Structure # <input checked="" type="checkbox"/>	Questel Orbit
Date Searcher Picked Up: <u>3/16/05</u>	Bibliographic	Dr Link
Date Completed: <u>3/16/05</u>	Integration	Lexis/Nexis
Searcher Prep & Review Time	Fulltext	Sequence Systems
Chemical Prep Time: <u>20</u>	Patent Family	WWW Internet
On-line Time: <u>145</u>	Other	Other (specify)

=> fil reg

FILE 'REGISTRY' ENTERED AT 08:31:34 ON 15 MAR 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7

DICTIONARY FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

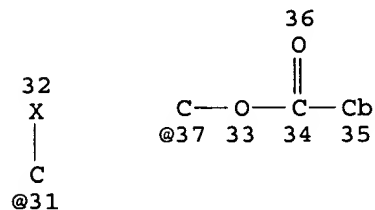
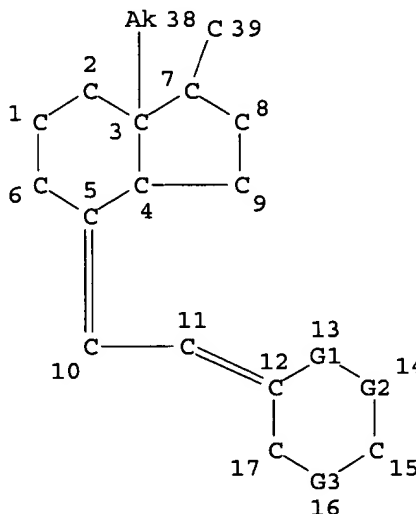
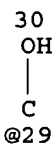
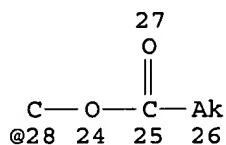
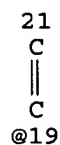
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d sta que l46

L15 1617 SEA FILE=REGISTRY ABB=ON PLU=ON (C5-C6 AND C6 AND C3)/ES

L17 STR



VAR G1=C/19

VAR G2=C/29/31/28/37

VAR G3=29/28/37

NODE ATTRIBUTES:

NSPEC IS RC AT 39

CONNECT IS M1 RC AT 39

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

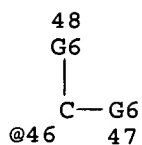
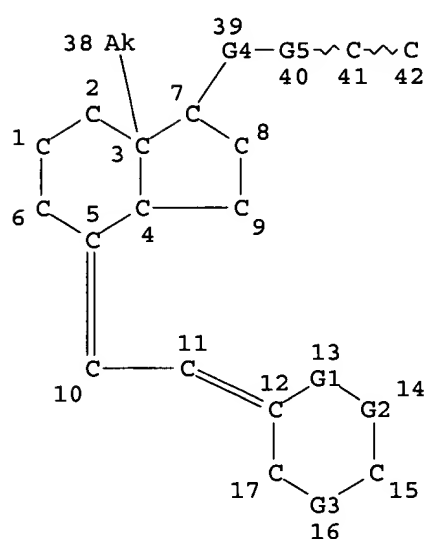
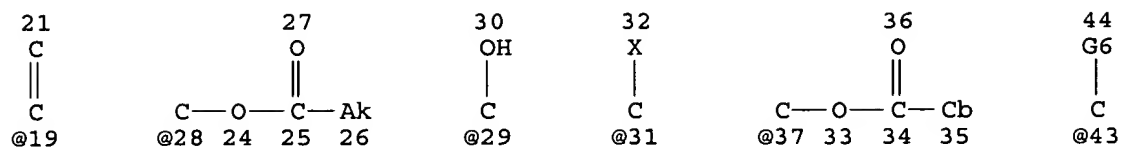
RSPEC 16 5

NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE

L19 907 SEA FILE=REGISTRY SUB=L15 CSS FUL L17

L24 STR



VAR G1=C/19
 VAR G2=C/29/31/28/37
 VAR G3=29/28/37
 VAR G4=C/43/46/19/CB
 VAR G5=C/29
 VAR G6=AK/X

NODE ATTRIBUTES:

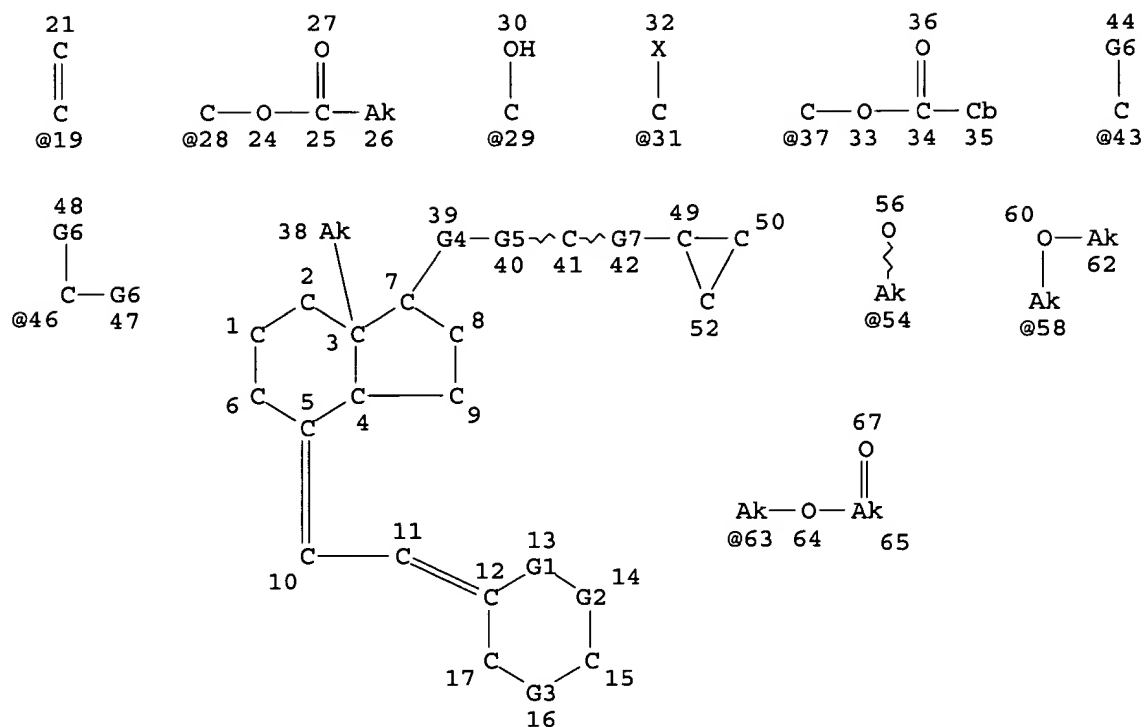
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 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 16 5
 NUMBER OF NODES IS 43

STEREO ATTRIBUTES: NONE

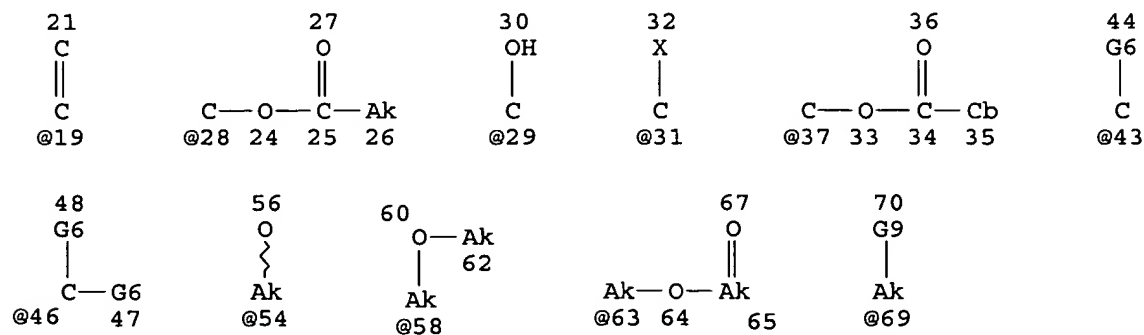
L26 881 SEA FILE=REGISTRY SUB=L19 CSS FUL L24
 L27 STR

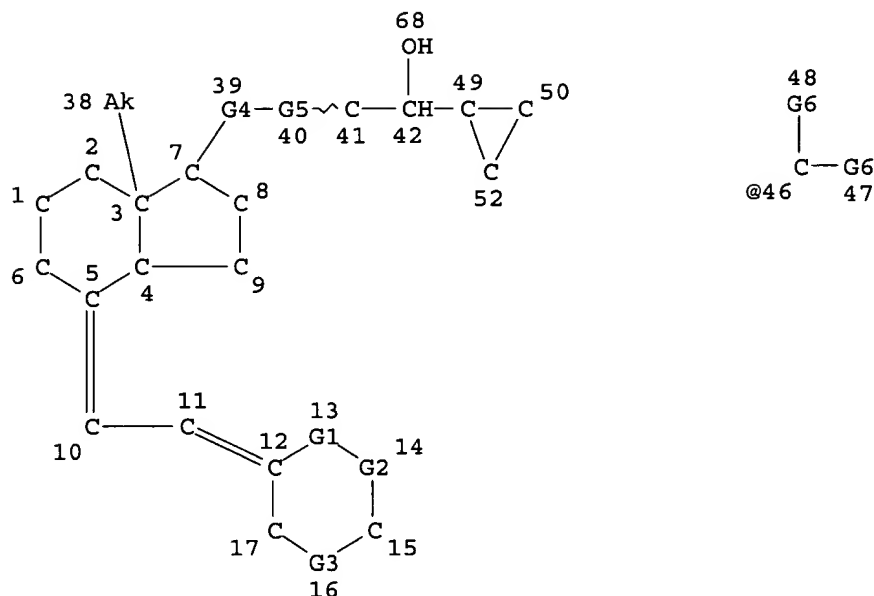
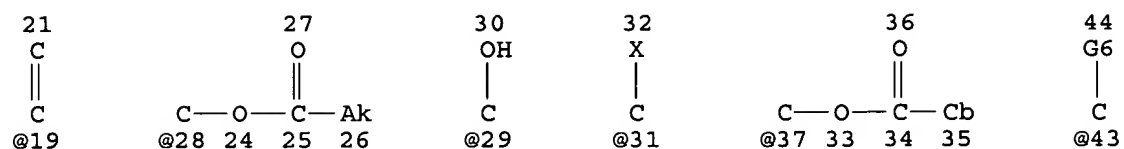


VAR G1=C/19
 VAR G2=C/29/31/28/37
 VAR G3=29/28/37
 VAR G4=C/43/46/19/CB
 VAR G5=C/29
 VAR G6=AK/X
 VAR G7=AK/54/58/63
 NODE ATTRIBUTES:
 CONNECT IS M1 RC AT 49
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RSPEC 7 12
 NUMBER OF NODES IS 55

STEREO ATTRIBUTES: NONE
 L29 742 SEA FILE=REGISTRY SUB=L26 CSS FUL L27
 L30 STR





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VAR G1=C/19
VAR G2=C/29/31/28/37
VAR G3=29/28/37
VAR G4=C/43/46/19/CB
VAR G5=C/29
VAR G6=AK/X
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 49
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

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GRAPH ATTRIBUTES:
RSPEC 7 12
NUMBER OF NODES IS 47

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STEREO ATTRIBUTES: NONE
L38      526 SEA FILE=REGISTRY SUB=L29 CSS FUL L36
L39      90  SEA FILE=REGISTRY ABB=ON  PLU=ON  L32 NOT L38
L41     216 SEA FILE=REGISTRY ABB=ON  PLU=ON  L29 NOT L38
L42     126 SEA FILE=REGISTRY ABB=ON  PLU=ON  L41 NOT L39
L43      84  SEA FILE=REGISTRY ABB=ON  PLU=ON  L42 AND NR>=5
L44     42  SEA FILE=REGISTRY ABB=ON  PLU=ON  L42 NOT L43
L45      7  SEA FILE=REGISTRY ABB=ON  PLU=ON  L44 AND (C32H39F9O4 OR
C35H52O5 OR C32H46O5 OR C34H39F13O4)
L46     97  SEA FILE=REGISTRY ABB=ON  PLU=ON  (L39 OR L45)

```

=> d his

(FILE 'HOME' ENTERED AT 07:50:14 ON 15 MAR 2005)
 SET COST OFF

FILE 'HCAPLUS' ENTERED AT 07:50:26 ON 15 MAR 2005

L1 1 S US20030018194/PN OR (US2002-214166# OR US2000-509934# OR WO98
E STEINMEYER A/AU
L2 47 S E3,E4
E NEEF G/AU
L3 186 S E3,E5-E7
E KIRSCH G/AU
L4 147 S E3-E5,E11
E SCHWARZ K/AU
L5 430 S E3-E14,E42,E43
E WIESINGER H/AU
L6 64 S E3-E6,E10
E HABEREY M/AU
L7 52 S E3,E4
E FAHNRICH M/AU
L8 7 S E3,E4
E FAEHNRICH M/AU
L9 7 S E3,E4
E LANGER G/AU
L10 238 S E3-E10,E19

FILE 'REGISTRY' ENTERED AT 07:53:16 ON 15 MAR 2005

FILE 'HCAPLUS' ENTERED AT 07:53:16 ON 15 MAR 2005

SET SMARTSELECT ON
L11 SEL L1 1- RN : 383 TERMS
SET SMARTSELECT OFF

FILE 'REGISTRY' ENTERED AT 07:53:16 ON 15 MAR 2005

L12 383 S L11
L13 250 S L12 AND C5-C6/ES AND C6/ES AND C3/ES
L14 STR
L15 1617 S (C5-C6 AND C6 AND C3)/ES
L16 37 S L14 CSS SAM SUB=L15
L17 STR L14
L18 37 S L17 CSS SAM SUB=L15
L19 907 S L17 CSS FUL SUB=L15
SAV L19 QAZI509/A
L20 143 S L12 AND L19
L21 107 S L13 NOT L20
L22 0 S L21 NOT SI/ELS
L23 0 S L20 AND NR>=5
L24 STR L17
L25 37 S L24 CSS SAM SUB=L19
L26 881 S L24 CSS FUL SUB=L19
SAV L26 QAZI509A/A
L27 STR L24
L28 30 S L27 CSS SAM SUB=L26
L29 742 S L27 CSS FUL SUB=L26
SAV L29 QAZI509B/A
L30 STR L27
L31 17 S L30 CSS SAM SUB=L29
L32 239 S L30 CSS FUL SUB=L29
SAV L32 QAZI509C/A
L33 143 S L12 AND L32
L34 96 S L32 NOT L33
L35 0 S L34 NOT 24() (DIHYDROXY OR TRIHYDROXY OR TRIOL)
L36 STR L27
L37 23 S L36 CSS SAM SUB=L29
L38 526 S L36 CSS FUL SUB=L29
SAV L38 QAZI509D/A
L39 90 S L32 NOT L38
L40 53 S L33 AND L38

L41 216 S L29 NOT L38
L42 126 S L41 NOT L39
L43 84 S L42 AND NR>=5
L44 42 S L42 NOT L43
L45 7 S L44 AND (C32H39F9O4 OR C35H52O5 OR C32H46O5 OR C34H39F13O4)
L46 97 S L39,L45
SAV L46 QAZI509E/A

FILE 'HCAOLD' ENTERED AT 08:30:04 ON 15 MAR 2005
L47 0 S L46

FILE 'HCAPLUS' ENTERED AT 08:30:09 ON 15 MAR 2005
L48 3 S L46
L49 3 S L48 AND L1-L10
L50 2 S L48 AND SCHERING?/PA,CS
L51 3 S L48-L50
L52 2 S L51 AND (PY<=1998 OR PRY<=1998 OR AY<=1998)
L53 3 S L51,L52

FILE 'USPATFULL' ENTERED AT 08:31:08 ON 15 MAR 2005
L54 3 S L46

FILE 'REGISTRY' ENTERED AT 08:31:34 ON 15 MAR 2005

=> fil uspatful

FILE 'USPATFULL' ENTERED AT 08:31:41 ON 15 MAR 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 10 Mar 2005 (20050310/PD)
FILE LAST UPDATED: 10 Mar 2005 (20050310/ED)
HIGHEST GRANTED PATENT NUMBER: US6865747
HIGHEST APPLICATION PUBLICATION NUMBER: US2005055750
CA INDEXING IS CURRENT THROUGH 10 Mar 2005 (20050310/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 10 Mar 2005 (20050310/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2005

>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d l54 bib abs hitrn fhitr tot

L54 ANSWER 1 OF 3 USPATFULL on STN

AN 2003:24350 USPATFULL
TI New Vitamin D derivatives with cyclopropyl rings in the side chains,
process and intermediate products for their production and their use for
the production of pharmaceutical agents
IN Steinmeyer, Andreas, Berlin, GERMANY, FEDERAL REPUBLIC OF
Neef, Gunter, Berlin, GERMANY, FEDERAL REPUBLIC OF
Kirsch, Gerald, Berlin, GERMANY, FEDERAL REPUBLIC OF
Schwarz, Kauca, Berlin, GERMANY, FEDERAL REPUBLIC OF
Wiesinger, Herbert, Berlin, GERMANY, FEDERAL REPUBLIC OF
Haberey, Martin, Berlin, GERMANY, FEDERAL REPUBLIC OF
Fahnrich, Marianne, Berlin, GERMANY, FEDERAL REPUBLIC OF
Langer, Gernot, Berlin, GERMANY, FEDERAL REPUBLIC OF
PI US 2003018194 A1 20030123
AI US 2002-214166 A1 20020808 (10)
RLI Continuation of Ser. No. US 2000-509934, filed on 3 May 2000, PENDING
PRAI DE 1997-19744127 19971001
DT Utility
FS APPLICATION
LREP MILLEN, WHITE, ZELANO & BRANIGAN, P.C., 2200 CLARENDON BLVD., SUITE
1400, ARLINGTON, VA, 22201
CLMN Number of Claims: 13
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 3697
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The invention relates to new vitamin D derivatives of general formula
(I), process for their production, intermediate products of the process
as well as the use for production of pharmaceutical agents.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 223107-10-6P 223107-11-7P 223107-15-1P
223107-16-2P 223107-20-8P 223107-21-9P
223107-25-3P 223107-30-0P 223107-31-1P
223107-35-5P 223107-36-6P 223107-70-8P
223107-71-9P 223107-75-3P 223107-76-4P
223107-80-0P 223107-81-1P 223107-85-5P
223107-86-6P 223107-90-2P 223107-91-3P
223107-95-7P 223107-96-8P 223108-12-1P
223108-13-2P 223108-20-1P 223108-21-2P
223108-27-8P 223108-33-6P 223108-39-2P
223109-04-4P 223109-05-5P 223109-08-8P
223109-09-9P 223109-12-4P 223109-15-7P
223109-22-6P 223109-89-5P 223109-95-3P
223110-01-8P 223110-21-2P 223110-30-3P
223110-37-0P 223110-44-9P 223110-54-1P
223110-64-3P 223110-80-3P 223110-95-0P
223111-01-1P 223111-11-3P 223111-22-6P
223111-31-7P 223111-41-9P 223111-46-4P
223111-53-3P 223111-57-7P 223111-62-4P
223111-67-9P 223111-73-7P 223111-80-6P
223111-86-2P 223111-89-5P 223111-94-2P
223111-97-5P 223112-01-4P 223112-04-7P
223112-06-9P 223112-10-5P 223112-13-8P
223112-15-0P 223112-17-2P 223112-18-3P
223112-19-4P 223112-20-7P 223112-21-8P
223112-23-0P 223112-25-2P 223112-27-4P
223112-28-5P 223112-31-0P 223112-35-4P
223112-39-8P 223112-43-4P 223112-48-9P
223112-52-5P 223112-54-7P 223112-57-0P
223112-60-5P 223112-63-8P
(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral
chains and pharmaceutical uses)
IT 223107-26-4P

(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral chains and pharmaceutical uses)

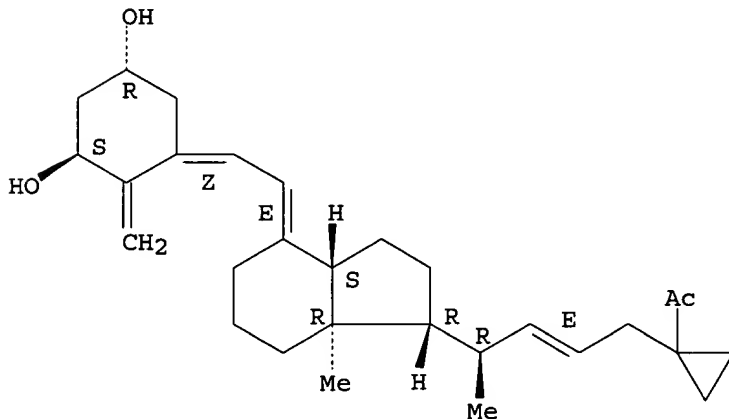
IT 223107-10-6P

(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral chains and pharmaceutical uses)

RN 223107-10-6 USPATFULL

CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



L54 ANSWER 2 OF 3 USPATFULL on STN

AN 2002:88470 USPATFULL

TI Vitamin D derivatives with substituents at C-25, process for their production, intermediate products and use for the production of pharmaceutical agents

IN Kirsch, Gerald, Berlin, GERMANY, FEDERAL REPUBLIC OF
Steinmeyer, Andreas, Berlin, GERMANY, FEDERAL REPUBLIC OF
Neef, Gunter, Berlin, GERMANY, FEDERAL REPUBLIC OF
Schwarz, Katica, Berlin, GERMANY, FEDERAL REPUBLIC OF
Thieroff-Ekerdt, Ruth, Berlin, GERMANY, FEDERAL REPUBLIC OF
Wiesinger, Herbert, Berlin, GERMANY, FEDERAL REPUBLIC OF
Menrad, Andreas, Berlin, GERMANY, FEDERAL REPUBLIC OF
Haberey, Martin, Berlin, GERMANY, FEDERAL REPUBLIC OF

PA Schering Aktiengesellschaft, Berlin, GERMANY, FEDERAL REPUBLIC OF (non-U.S. corporation)

PI US 6376480 B1 20020423

AI US 2000-738286 20001218 (9)

RLI Continuation of Ser. No. US 981819

PRAI DE 1995-19522797 19950614

DT Utility

FS GRANTED

EXNAM Primary Examiner: Pryor, Alton

LREP Millen, White, Zelano & Branigan, P.C.

CLMN Number of Claims: 17

ECL Exemplary Claim: 1

DRWN 0 Drawing Figure(s); 0 Drawing Page(s)

LN.CNT 2658

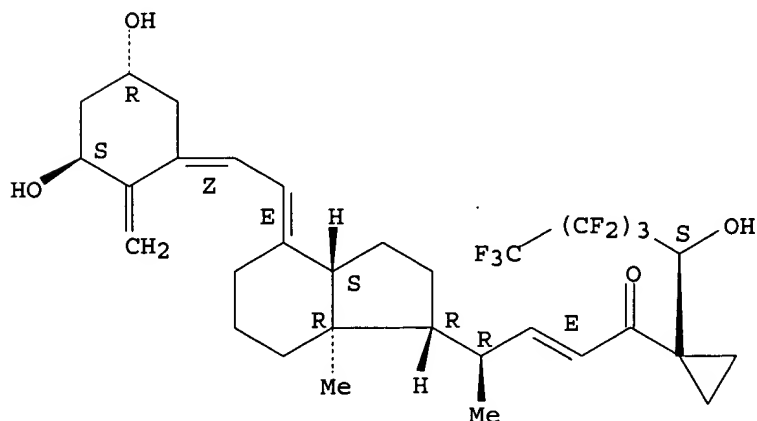
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A method of preparing a pharmaceutical composition, comprising combining a pharmaceutically compatible vehicle with a compound according to formula (I) ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 186373-06-8P 186373-07-9P 186374-00-5P
 186374-01-6P 186374-16-3P 186374-17-4P
 (preparation of 25-substituted vitamin D derivs. with antiproliferative activity)
 IT 186373-06-8P
 (preparation of 25-substituted vitamin D derivs. with antiproliferative activity)
 RN 186373-06-8 USPATFULL
 CN 9,10-Secochola-5,7,10(19),22-tetraen-24-one, 1,3-dihydroxy-24-[1-(2,2,3,3,4,4,5,5,5-nonafluoro-1-hydroxypentyl)cyclopropyl]-, [1 α ,3 β ,5Z,7E,22E,24(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.



L54 ANSWER 3 OF 3 USPATFULL on STN
 AN 2002:81475 USPATFULL
 TI Vitamin D derivatives with C-25 substituents, process for their preparation, intermediate products and their use in preparing medicaments
 IN Kirsch, Gerald, Berlin, GERMANY, FEDERAL REPUBLIC OF
 Steinmeyer, Andreas, Berlin, GERMANY, FEDERAL REPUBLIC OF
 Neef, Gunter, Berlin, GERMANY, FEDERAL REPUBLIC OF
 Schwarz, Katica, Berlin, GERMANY, FEDERAL REPUBLIC OF
 Thieroff-Ekerdt, Ruth, Berlin, GERMANY, FEDERAL REPUBLIC OF
 Wiesinger, Herbert, Berlin, GERMANY, FEDERAL REPUBLIC OF
 Menrad, Andreas, Berlin, GERMANY, FEDERAL REPUBLIC OF
 Haberey, Martin, Berlin, GERMANY, FEDERAL REPUBLIC OF
 PA Schering Aktiengesellschaft, Berlin, GERMANY, FEDERAL REPUBLIC OF (non-U.S. corporation)
 PI US 6372731 B1 20020416
 WO 9700242 19970103
 AI US 1998-981819 19980331 (8)
 WO 1996-EP1788 19960430
 19980331 PCT 371 date
 PRAI DE 1995-19522797 19950614
 DT Utility
 FS GRANTED
 EXNAM Primary Examiner: Dees, Jose' G.; Assistant Examiner: Pryor, Alton
 LREP Millen, White, Zelano & Branigan, P.C.
 CLMN Number of Claims: 6
 ECL Exemplary Claim: 1
 DRWN 14 Drawing Figure(s); 14 Drawing Page(s)
 LN.CNT 2853
 CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A vitamin D derivative and its uses with substituents at C-25 of general formula I ##STR1##

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 186373-06-8P 186373-07-9P 186374-00-5P
186374-01-6P 186374-16-3P 186374-17-4P

(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

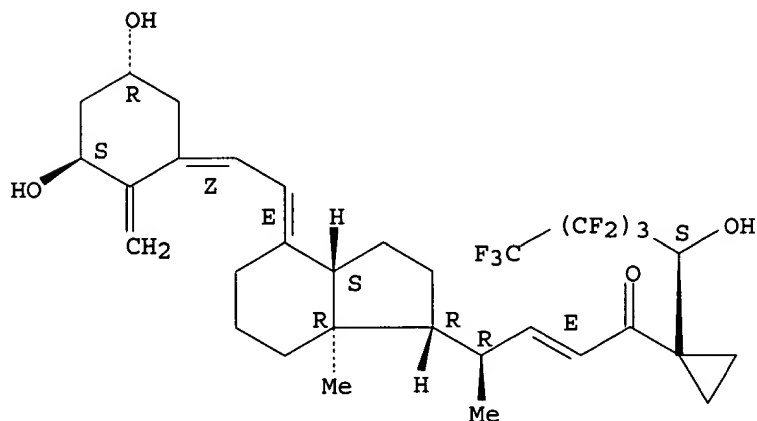
IT 186373-06-8P

(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

RN 186373-06-8 USPATFULL

CN 9,10-Secochola-5,7,10(19),22-tetraen-24-one, 1,3-dihydroxy-24-[1-(2,2,3,3,4,4,5,5,5-nonafluoro-1-hydroxypentyl)cyclopropyl]-, [1 α ,3 β ,5 ζ ,7 ϵ ,22 ϵ ,24(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 08:31:50 ON 15 MAR 2005

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FILE COVERS 1907 - 15 Mar 2005 VOL 142 ISS 12

FILE LAST UPDATED: 14 Mar 2005 (20050314/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l53 all hitstr tot

L53 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:776356 HCAPLUS
DN 134:65808
ED Entered STN: 06 Nov 2000
TI Structure activity relationship of carboxylic ester antagonists of the vitamin D3 receptor
AU Bury, Yvonne; **Steinmeyer, Andreas**; Carlberg, Carsten
CS Institut fur Physiologische Chemie I and Biomedizinisches Forschungszentrum, Heinrich-Heine-Universitat, Dusseldorf, Germany
SO Molecular Pharmacology (2000), 58(5), 1067-1074
CODEN: MOPMA3; ISSN: 0026-895X
PB American Society for Pharmacology and Experimental Therapeutics
DT Journal
LA English
CC 1-3 (Pharmacology)
Section cross-reference(s): 2
AB A 25-carboxylic ester analog of $1\alpha,25$ -dihydroxyvitamin D3 [$1\alpha,25(\text{OH})_2\text{D}_3$], ZK159222, was recently described as a novel type of antagonist of $1\alpha,25(\text{OH})_2\text{D}_3$ signaling. In this study five derivs. of ZK159222 were selected because of their sensitivity in facilitating complex formation between the $1\alpha,25(\text{OH})_2\text{D}_3$ receptor (VDR) and the retinoid X receptor on a $1\alpha,25(\text{OH})_2\text{D}_3$ response element that was comparable to that of the natural hormone (0.2-0.9 nM). Most derivs. of ZK159222 reacted as typical agonists, because they were able to promote ligand-dependent interaction of the VDR with the coactivator TIF2, stabilized the VDR preferentially in its agonistic conformation c1LPD, and stimulated VDR-dependent gene activity with a potency similar to $1\alpha,25(\text{OH})_2\text{D}_3$. In contrast, only one derivative showed the antagonistic profile of ZK159222, which includes the incompetence to induce a VDR-TIF2 contact, the stabilization of the antagonistic conformation c2LPD, and only a very weak and insensitive functional activity. Accordingly, ZK159222 and only one of its derivative showed prominent antagonistic effects in cellular systems. The comparison of the structures of the compds. indicates that the essential requirements for an antagonistic function are a cyclopropyl ring at carbon 25, a hydroxy group at carbon 24, and at least a Bu ester. Interestingly, the active derivative was approx. 3 times more sensitive antagonist than ZK159222 and even displayed a lower residual agonistic activity. In conclusion, only a very limited number of structural variations of ZK159222 are possible to keep its antagonistic profile, but the tools presented here for their in vitro evaluation allow an accurate prediction of the effects and are suited to screening for even more potent $1\alpha,25(\text{OH})_2\text{D}_3$ antagonists.
ST vitamin D3 receptor antagonist ZK159222 conformation; structure activity ZK159222 analogs retinoid x receptor
IT Conformation
(protein, c1LPD and c2LPD; structure activity relationship of carboxylic ester antagonists of vitamin D3 receptor)
IT Structure-activity relationship
(structure activity relationship of carboxylic ester antagonists of vitamin D3 receptor)
IT Retinoid X receptors
Vitamin D receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(structure activity relationship of carboxylic ester antagonists of vitamin D3 receptor)
IT 32222-06-3, $1\alpha,25(\text{OH})_2\text{D}_3$ 156965-15-0, ZK159222 163207-55-4
186371-96-0 316187-11-8 316187-12-9 **316187-13-0**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(structure activity relationship of carboxylic ester antagonists of vitamin D3 receptor)

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

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IT 316187-13-0

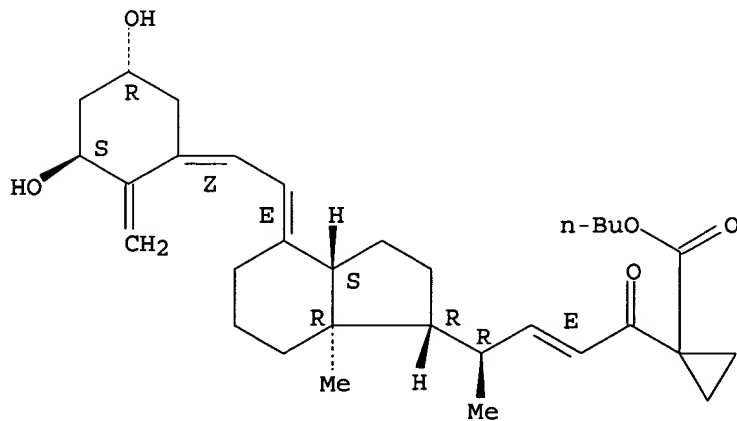
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(structure activity relationship of carboxylic ester antagonists of vitamin D3 receptor)

RN 316187-13-0 HCAPLUS

CN Cyclopropanecarboxylic acid, 1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-24-oxo-9,10-secochola-5,7,10(19),22-tetraen-24-yl]-, butyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



DN 130:296893
 ED Entered STN: 15 Apr 1999
 TI Preparation of novel vitamin D derivatives with cyclopropyl ring in the lateral chains and their pharmaceutical uses
 IN Steinmeyer, Andreas; Neef, Gunter; Kirsch, Gerald; Schwarz, Katica; Wiesinger, Herbert; Haberey, Martin; Fahnrich, Marianne; Langer, Gernot
 PA Schering A.-G., Germany
 SO PCT Int. Appl., 130 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 IC ICM C07C401-00
 ICS A61K031-59
 CC 32-7 (Steroids)
 Section cross-reference(s): 1, 2, 63

FAN.CNT 1

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PI	WO 9916745	A1	19990408	WO 1998-EP6159	19980929 <--
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	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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	CA 2305140	AA	19990408	CA 1998-2305140	19980929 <--
	AU 9911476	A1	19990423	AU 1999-11476	19980929 <--
	AU 750011	B2	20020711		
	EP 1025082	A1	20000809	EP 1998-954292	19980929 <--
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	ES 2199472	T3	20040216	ES 1998-954292	19980929 <--
	US 2003018194	A1	20030123	US 2002-214166	20020808 <--
PRAI	DE 1997-19744127	A	19971001	<--	
	WO 1998-EP6159	W	19980929	<--	
	US 2000-509934	A1	20000503	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9916745	ICM	C07C401-00
	ICS	A61K031-59
WO 9916745	ECLA	A61K031/59+M; A61K038/13+M; A61K039/395+M; C07C401/00
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DE 19744127	ECLA	A61K031/59+M; A61K038/13+M; A61K039/395+M; C07C401/00
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US 2003018194	ECLA	A61K031/59+M; A61K038/13+M; A61K039/395+M; C07C401/00
		<--

OS MARPAT 130:296893

GI

AB The title compds. [I; Y1 = H, OH, F, Cl, Br, hydrocarbylcarbonyloxy; Y2 = H, hydrocarbylcarbonyl; R1, R2 = H, or R1R2 = CH2; R3, R4 = H, Cl, F, alkyl, or R3R4 = CH2, or R3R4C = carbocyclic ring; VW = bond, or V = OH and W = H; Q = hydrocarbyl optionally possessing OH which may be etherified or esterified, CO, NH2, halo; Z = hydrocarbyl optionally possessing CO, OH which may be etherified or esterified, NH2, F, Cl, Br], useful for treating disorders such as calcium absorption disorders, hyperproliferative skin disorders, pruritus, tumors, immunol. disorders, inflammation, rheumatoid arthritis, asthma, autoimmune diseases, multiple sclerosis, diabetes mellitus, AIDS, as well as rejection in organ transplantation, are prepared Thus, sulfone II (also prepared) was reacted with III (also prepared) in THF containing diisopropylamine and BuLi to give, after elimination reaction and deprotection, the title compound IV. This had an affinity to the calcitriol receptor comparable to that of calcitriol.

ST vitamin D deriv cyclopropane ring prepn; calcium vitamin D deriv cyclopropane ring

IT Skin, disease
(hyperproliferative; preparation of novel vitamin D derivs. with cyclopropyl ring in lateral chains and pharmaceutical uses)

IT Anti-AIDS agents
Anti-inflammatory agents
Antiasthmatics
Antidiabetic agents
Antitumor agents
Autoimmune disease
Immunomodulators
Multiple sclerosis
Pruritus
Rheumatoid arthritis
(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral chains and pharmaceutical uses)

IT Transplant and Transplantation
(rejection, drugs for; preparation of novel vitamin D derivs. with cyclopropyl ring in lateral chains and pharmaceutical uses)

IT 223107-10-6P 223107-11-7P 223107-15-1P
223107-16-2P 223107-20-8P 223107-21-9P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral chains and pharmaceutical uses)

IT 75-03-6, Iodoethane 104-15-4, reactions 105-45-3, Methyl acetoacetate 106-93-4, 1,2-Dibromoethane 107-08-4, 1-Iodopropane 107-21-1, 1,2-Ethanediol, reactions 108-98-5, Thiophenol, reactions 542-69-8, 1-Iodobutane 628-17-1, 1-Iodopentane 638-45-9, 1-Iodohexane 4202-14-6 4762-26-9, Hexyltriphenylphosphonium bromide 5927-18-4, Methyl dimethylphosphonoacetate 6228-47-3, Propyltriphenylphosphonium bromide 13423-48-8, Heptyltriphenylphosphonium bromide 21406-61-1, Pentyltriphenylphosphonium bromide 112828-13-4 223109-38-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral chains and pharmaceutical uses)

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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral
chains and pharmaceutical uses)

IT 7440-70-2, Calcium, biological studies

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
(Biological study); PROC (Process)

(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral
chains for calcium absorption regulation)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

- (1) Leo Pharmaceutical Products Ltd; WO 8910351 A 1989 HCAPLUS
- (2) Leo Pharmaceutical Products Ltd; WO 8700834 A 1987 HCAPLUS
- (3) Schering Ag; WO 9700242 A 1997 HCAPLUS

IT 223107-10-6P 223107-11-7P 223107-15-1P

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RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)

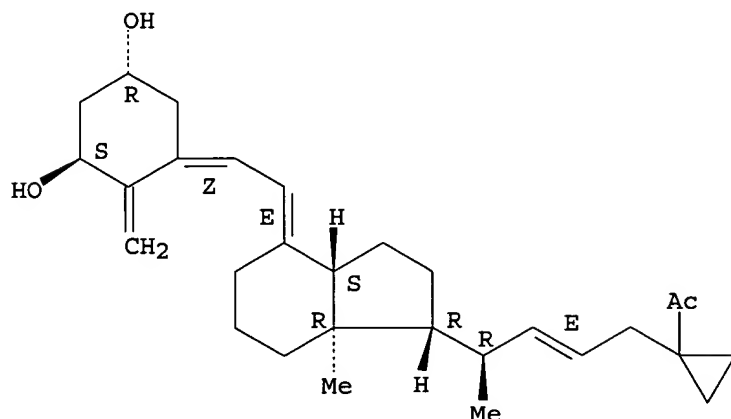
(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral
chains and pharmaceutical uses)

RN 223107-10-6 HCAPLUS

CN Ethanone, 1- [1- [(1 α , 3 β , 5Z, 7E, 22E) -1, 3-dihydroxy-9, 10-secochola-

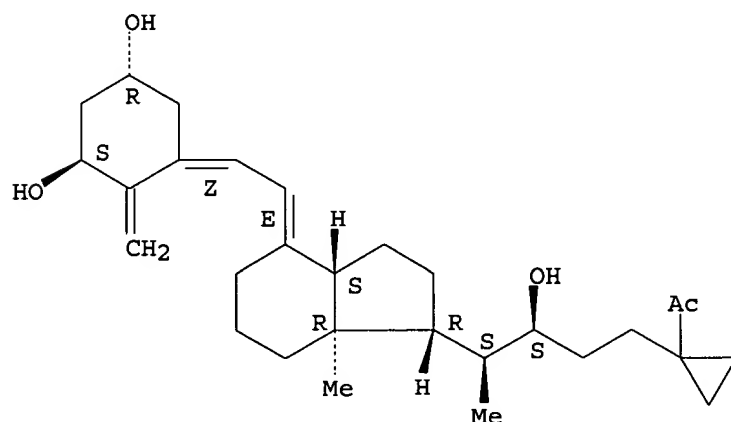
5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



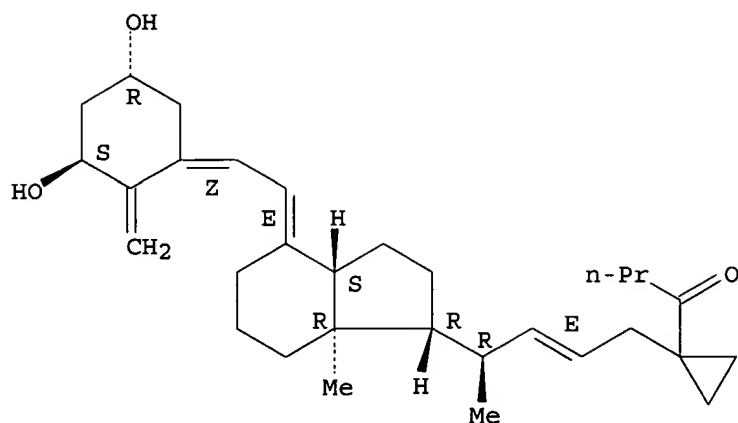
RN 223107-11-7 HCAPLUS
CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-15-1 HCAPLUS
CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

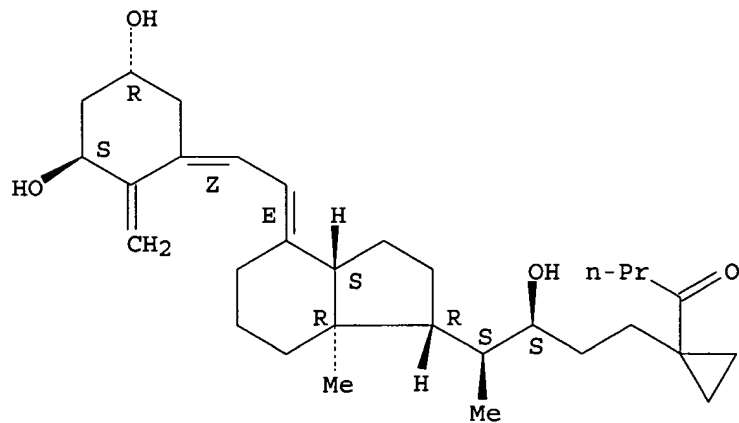
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-16-2 HCAPLUS

CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

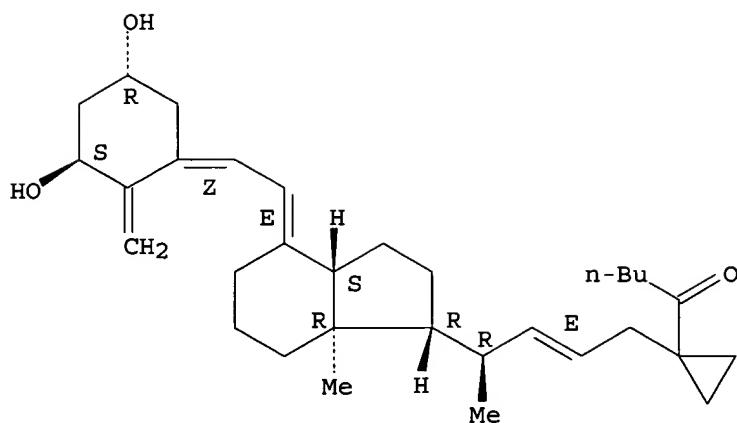
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-20-8 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

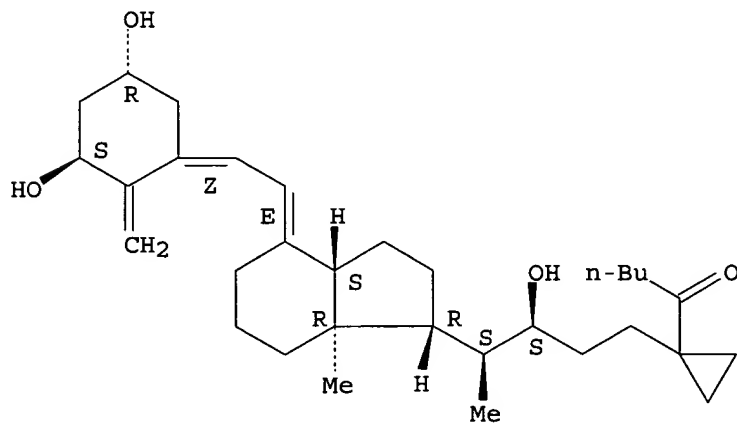
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-21-9 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

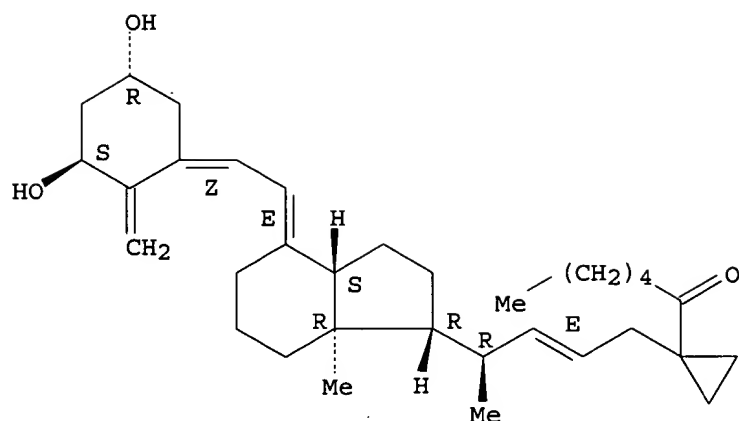
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-25-3 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

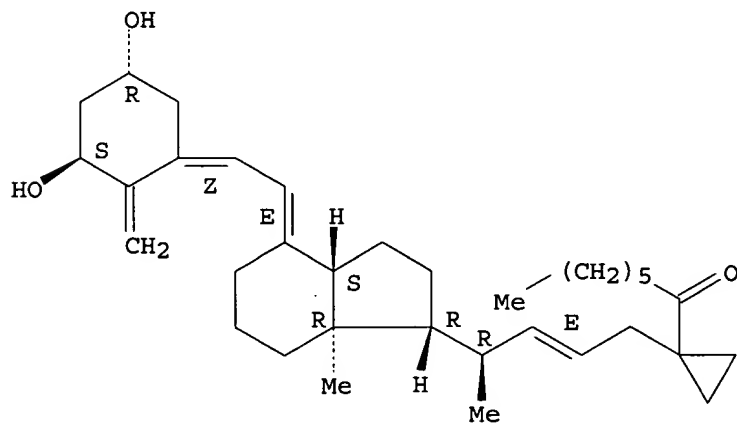
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-30-0 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

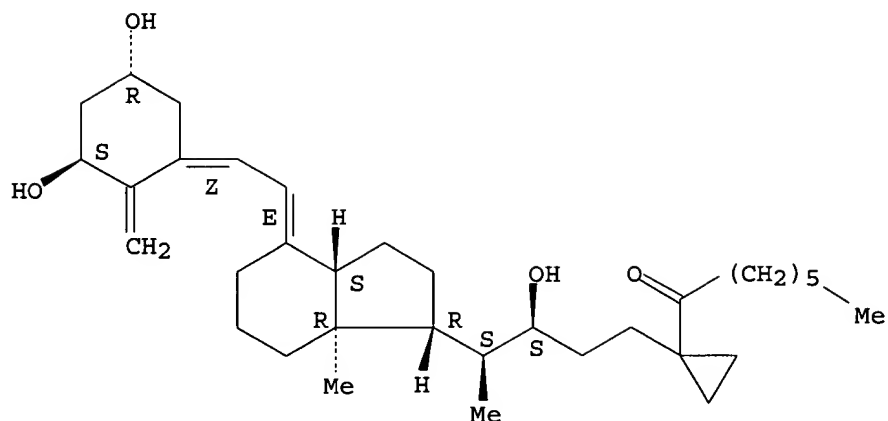
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-31-1 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

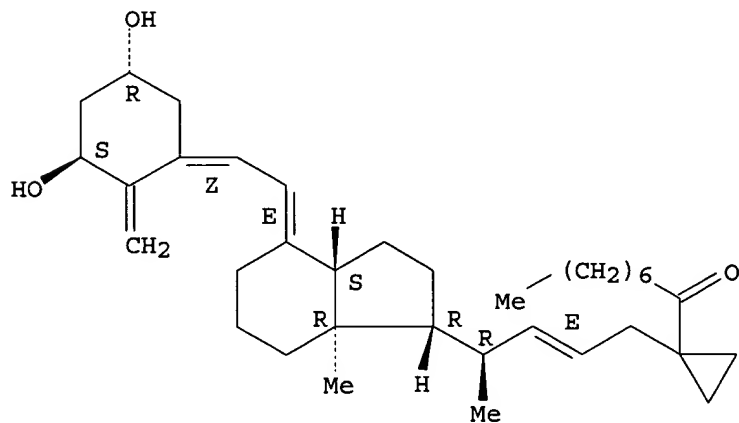
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-35-5 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

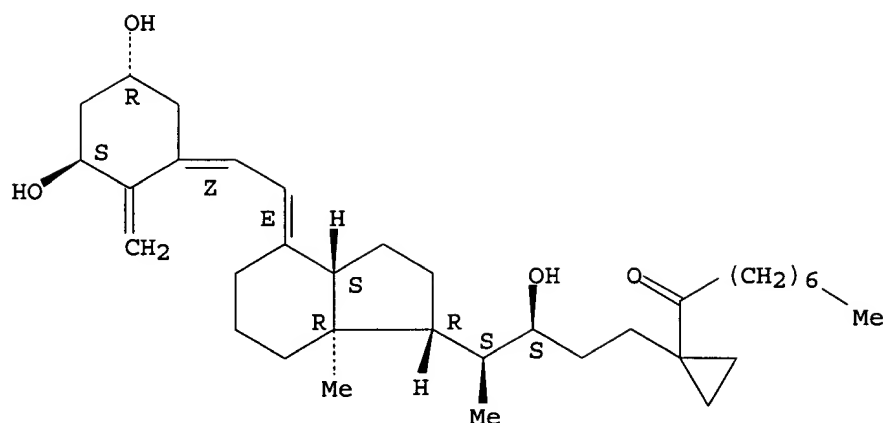
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-36-6 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

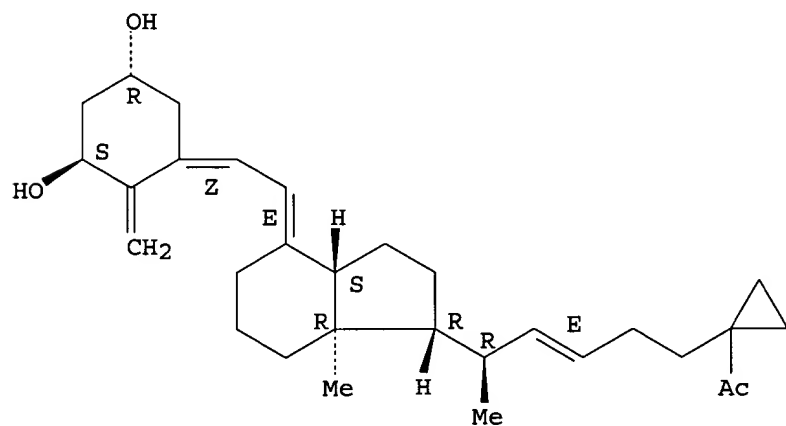
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-70-8 HCAPLUS

CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

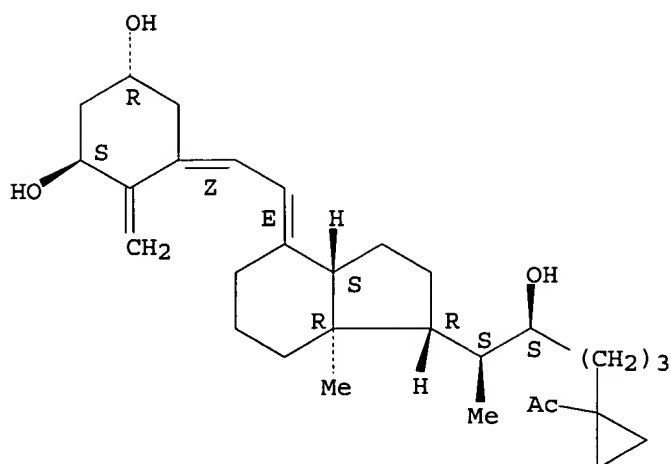
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-71-9 HCAPLUS

CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

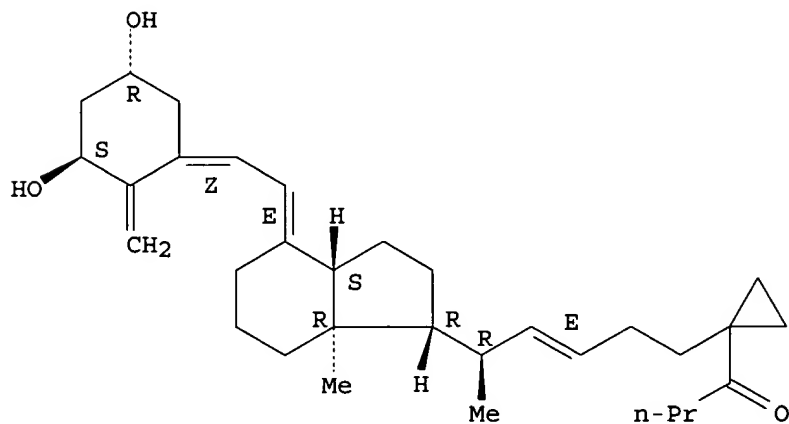
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-75-3 HCAPLUS

CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

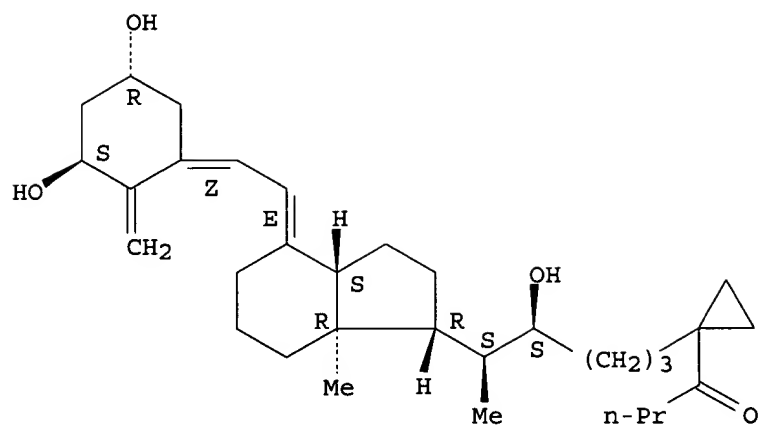
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-76-4 HCAPLUS

CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

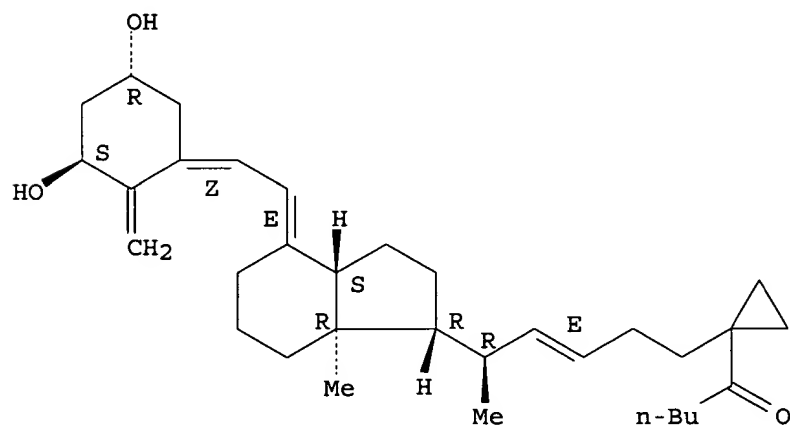
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-80-0 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

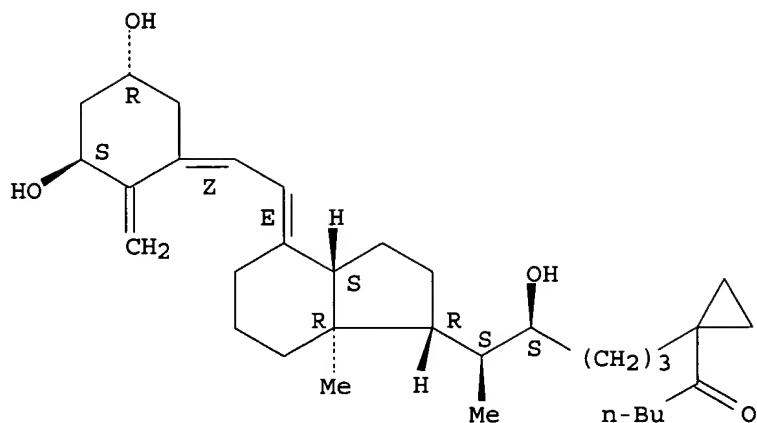
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-81-1 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

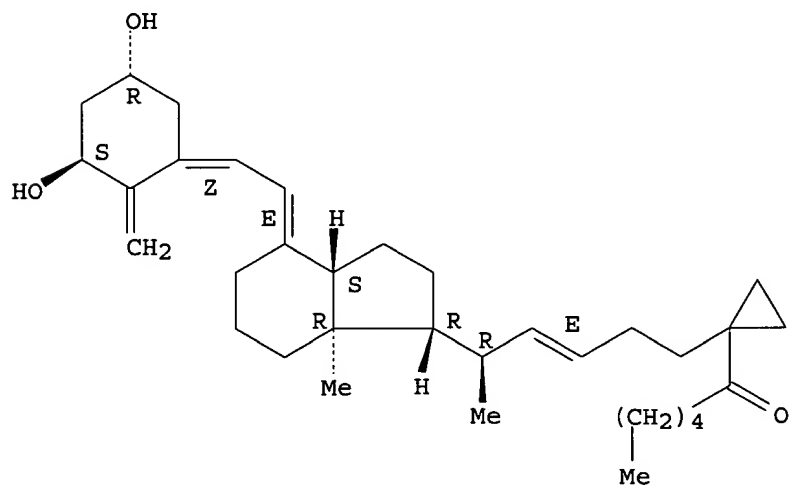
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-85-5 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

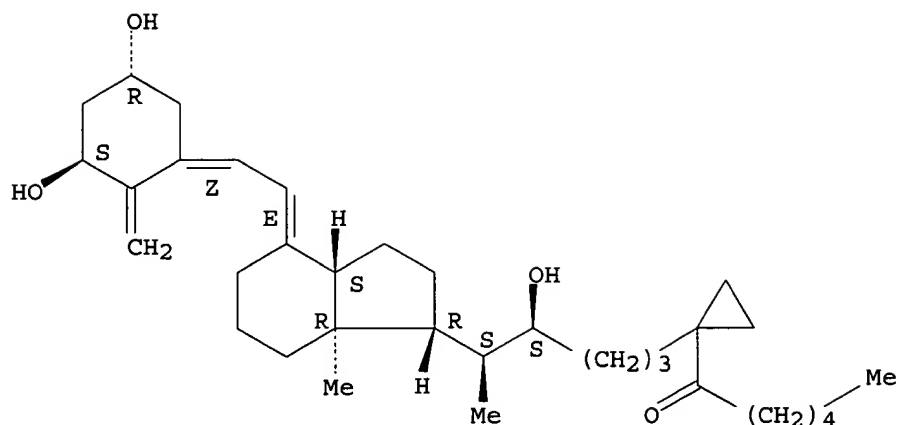
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-86-6 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

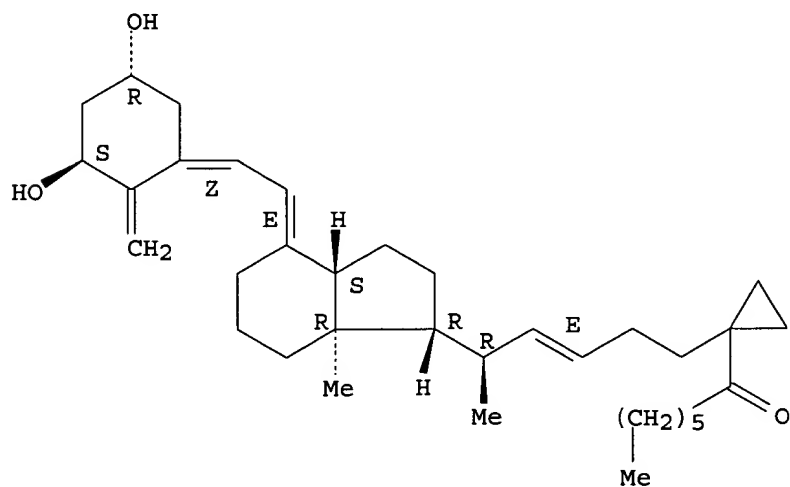
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-90-2 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

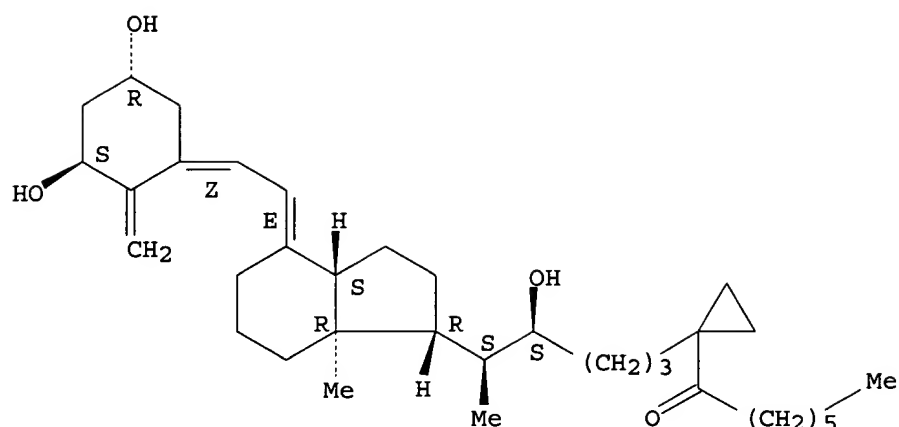
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-91-3 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

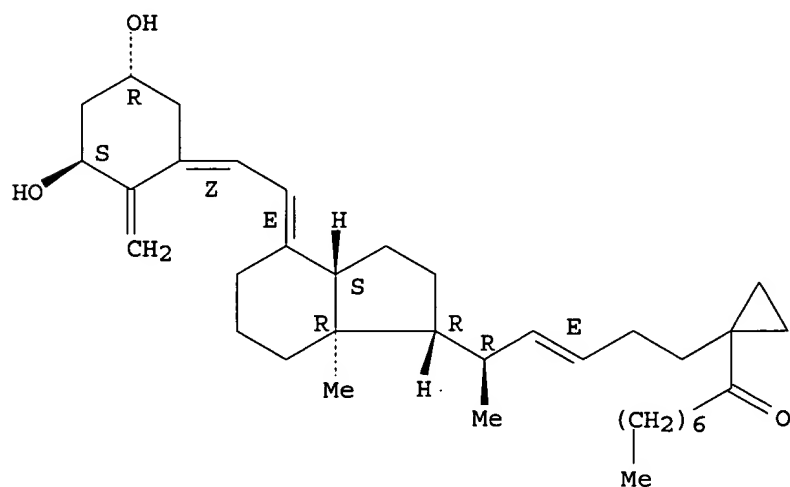
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-95-7 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

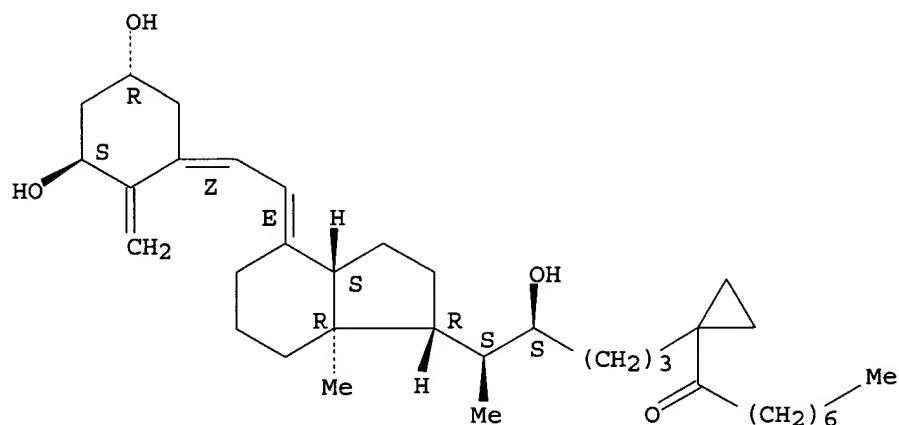
Absolute stereochemistry.
Double bond geometry as shown.



RN 223107-96-8 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

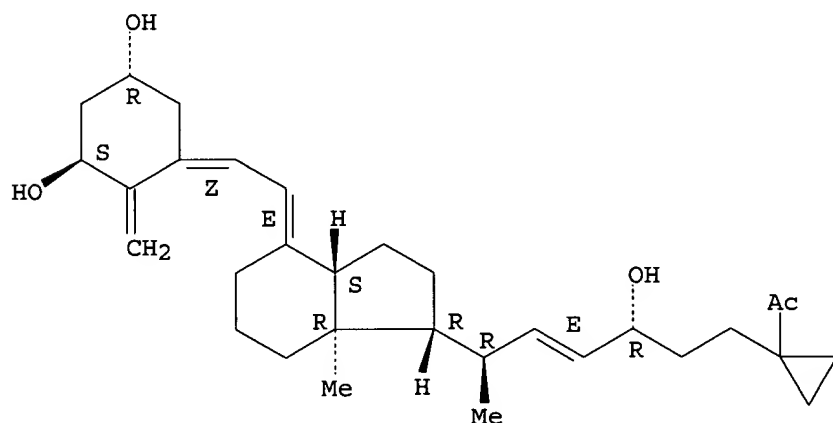
Absolute stereochemistry.
Double bond geometry as shown.



RN 223108-12-1 HCAPLUS

CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

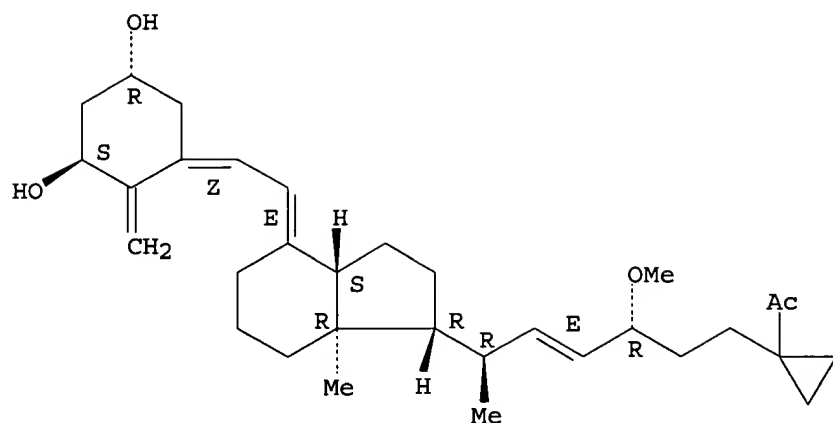
Absolute stereochemistry.
Double bond geometry as shown.



RN 223108-13-2 HCAPLUS

CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

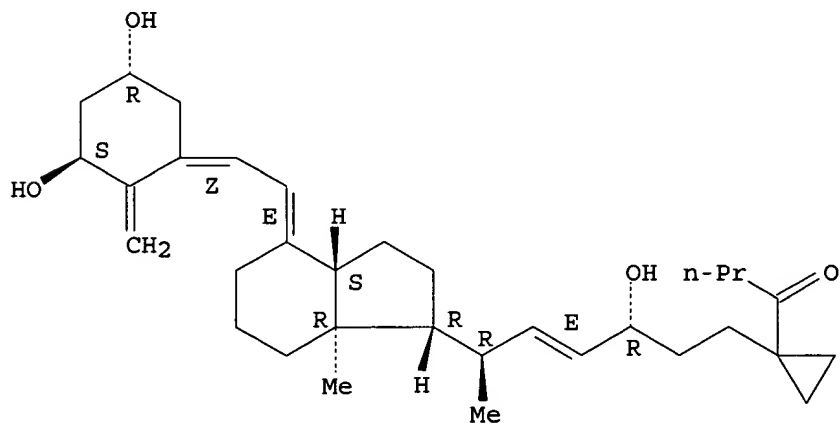
Absolute stereochemistry.
Double bond geometry as shown.



RN 223108-20-1 HCAPLUS

CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

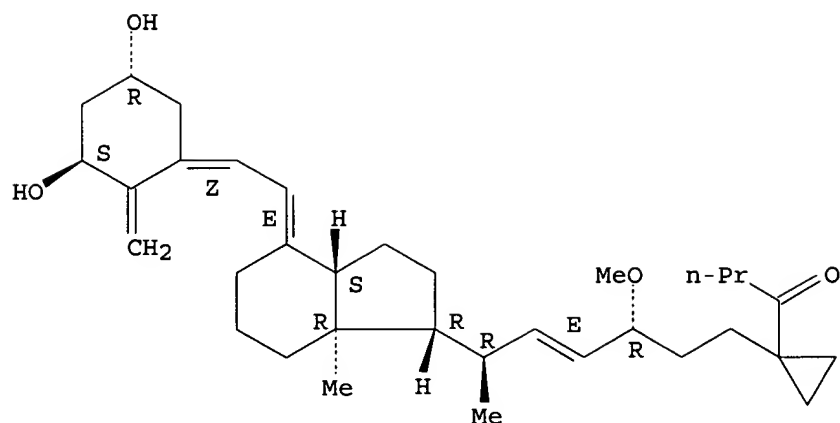
Absolute stereochemistry.
Double bond geometry as shown.



RN 223108-21-2 HCAPLUS

CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

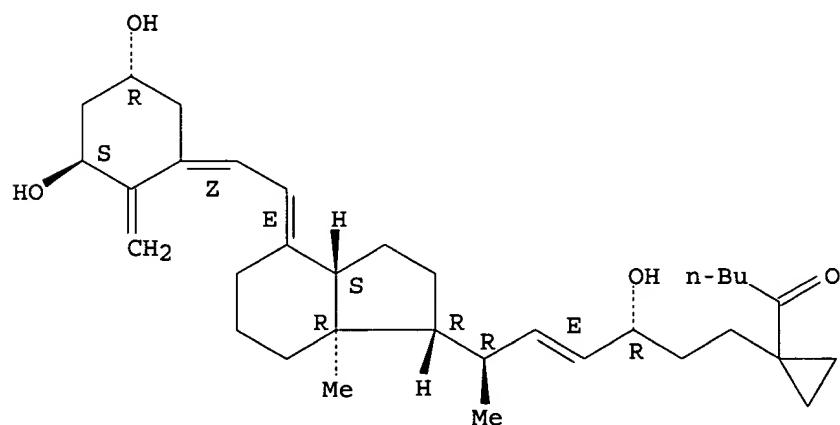
Absolute stereochemistry.
Double bond geometry as shown.



RN 223108-27-8 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

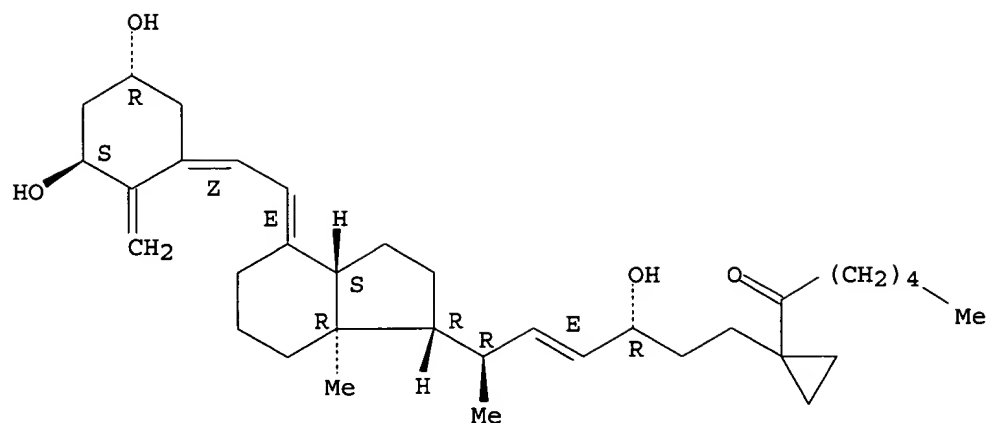
Absolute stereochemistry.
Double bond geometry as shown.



RN 223108-33-6 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

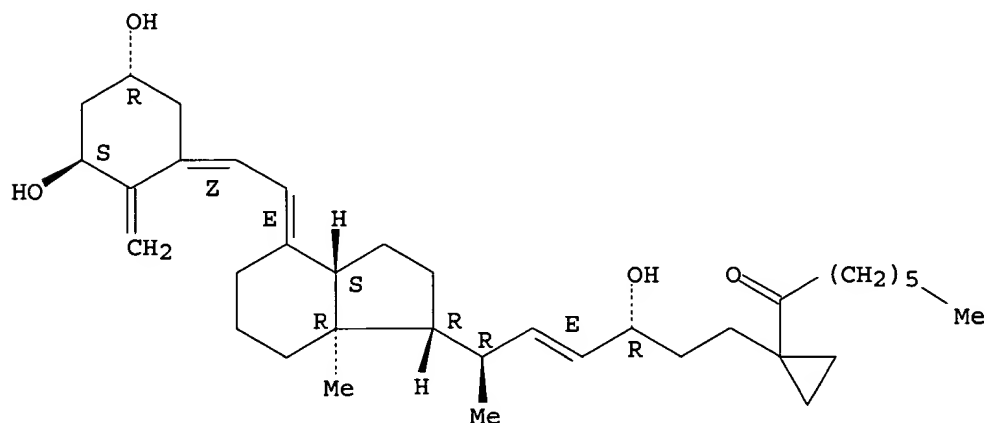
Absolute stereochemistry.
Double bond geometry as shown.



RN 223108-39-2 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

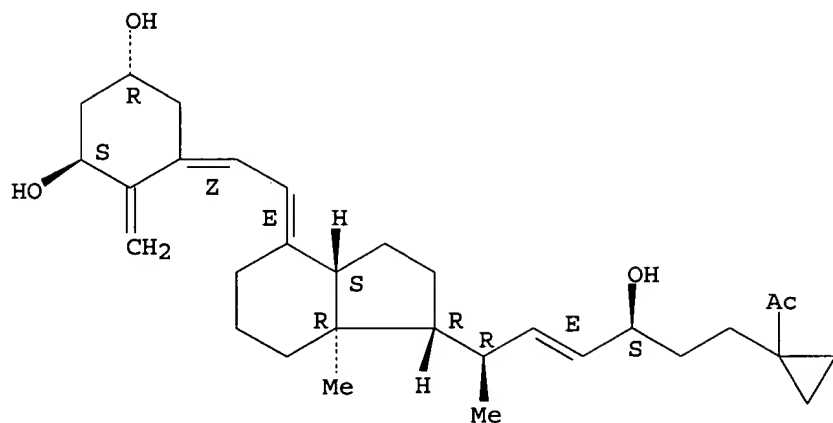
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-04-4 HCAPLUS

CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

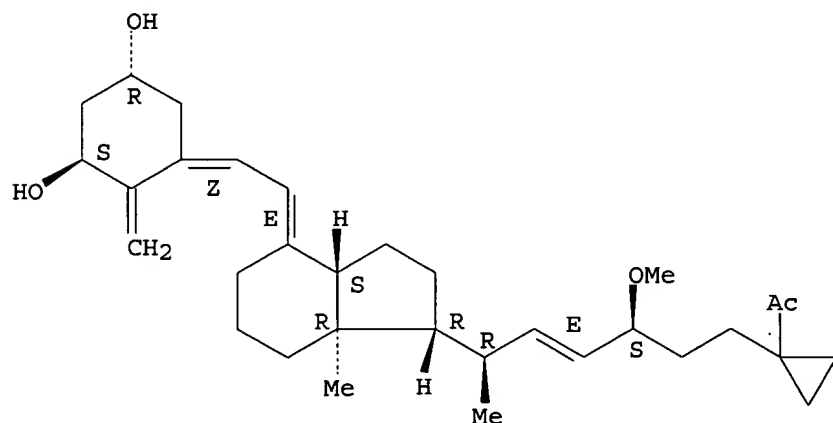
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-05-5 HCAPLUS

CN Ethanone, 1- [1- [(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl] - (9CI)
(CA INDEX NAME)

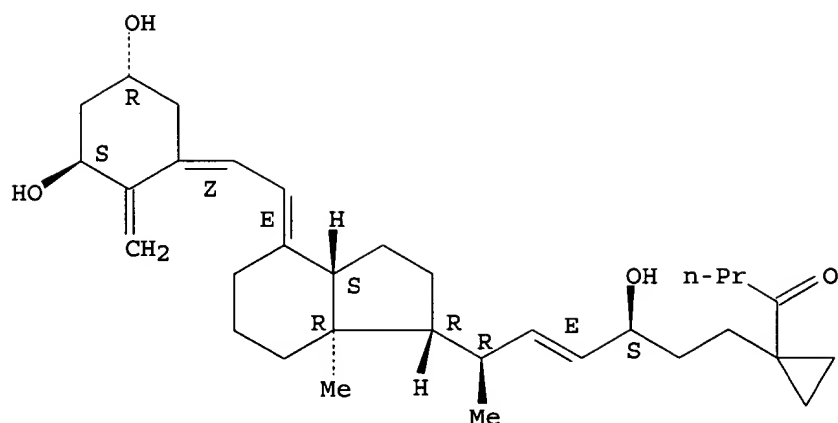
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-08-8 HCAPLUS

CN 1-Butanone, 1- [1- [(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl] - (9CI) (CA INDEX NAME)

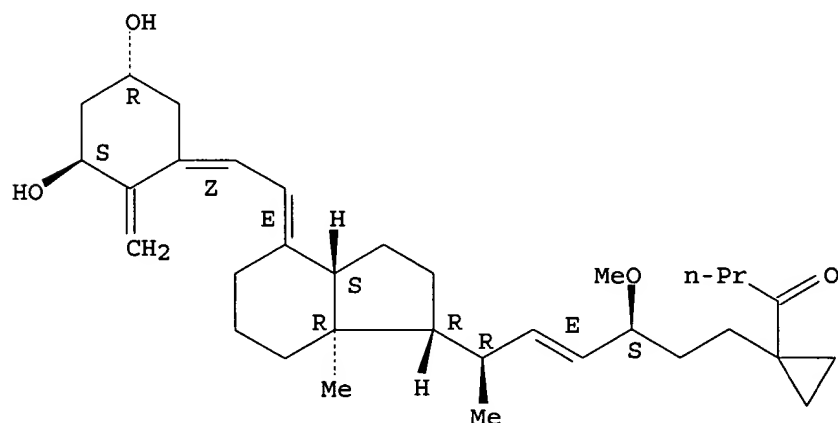
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-09-9 HCAPLUS

CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

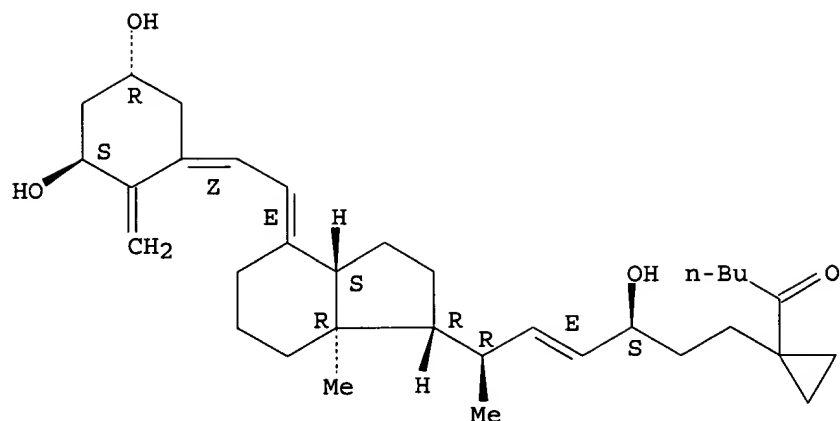
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-12-4 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

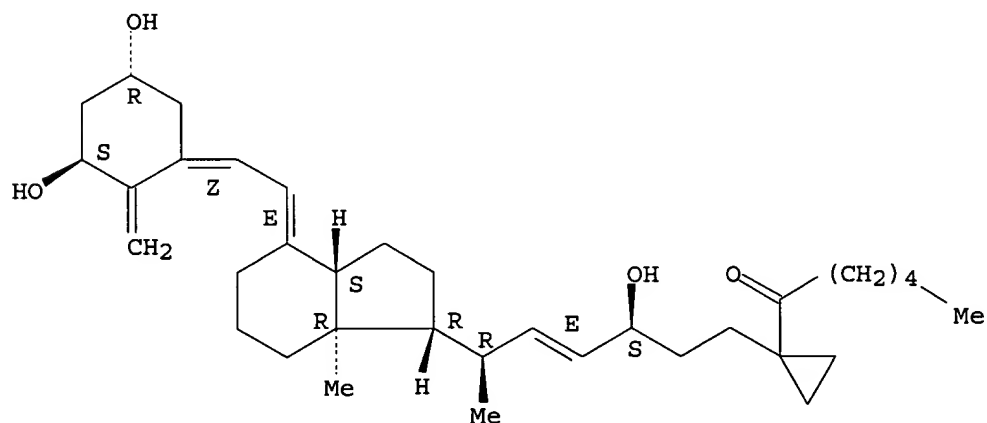
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-15-7 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

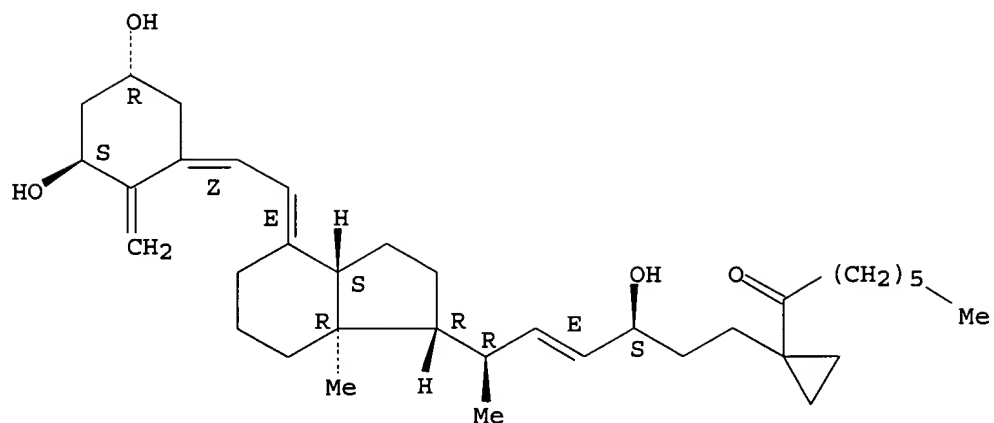
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-22-6 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

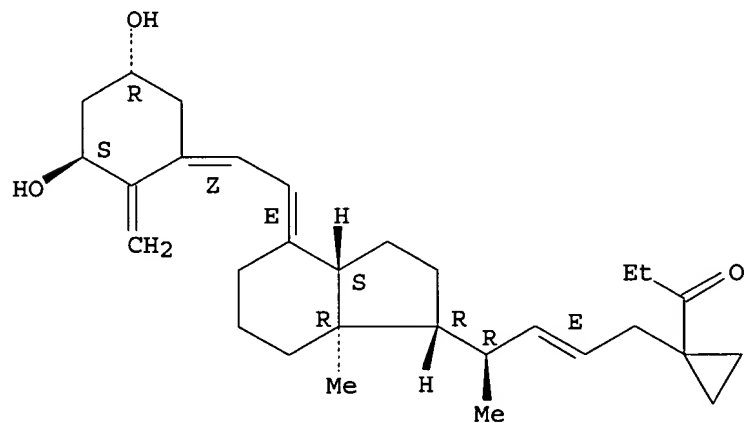
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-89-5 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

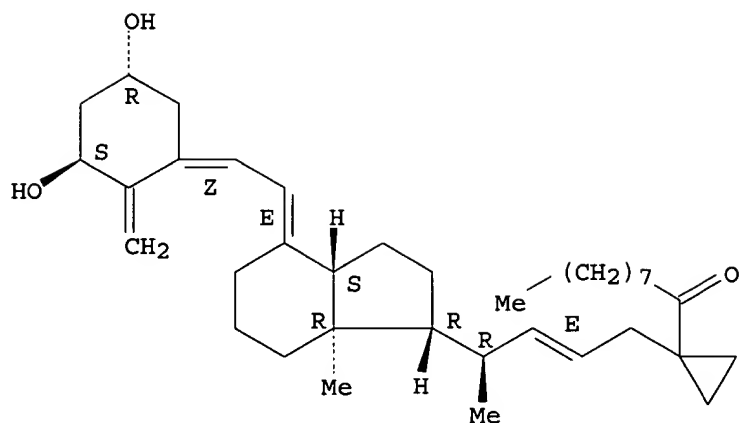
Absolute stereochemistry.
Double bond geometry as shown.



RN 223109-95-3 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

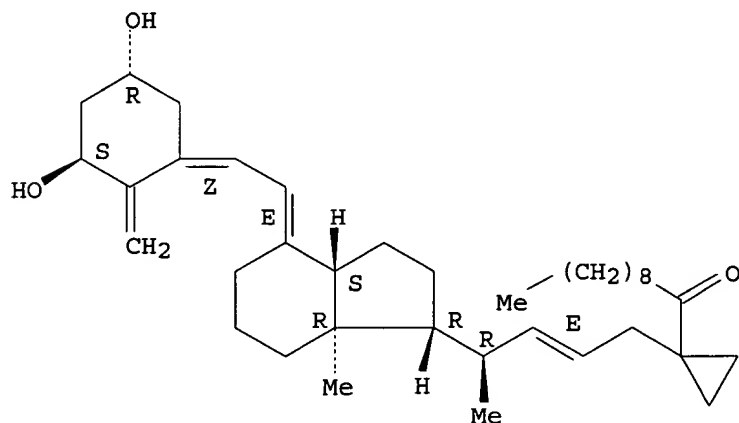
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-01-8 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

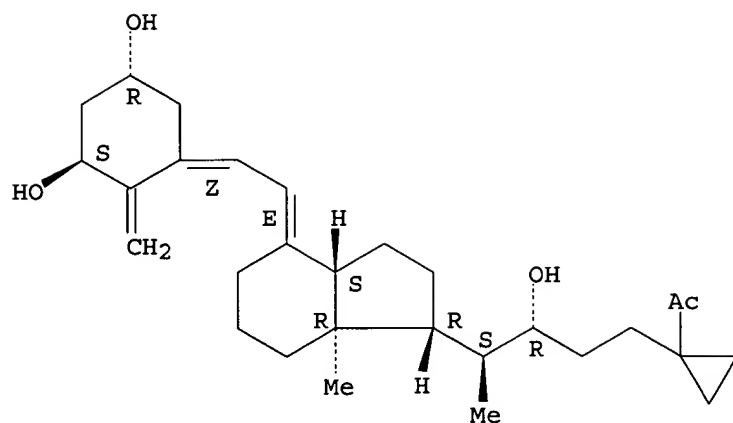
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-21-2 HCAPLUS

CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

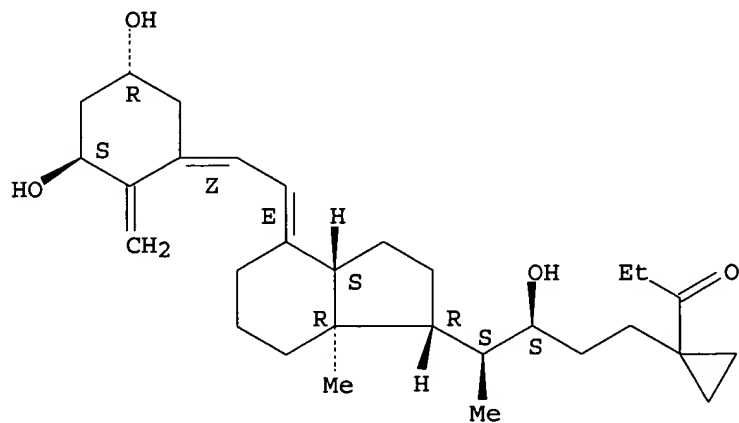
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-30-3 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

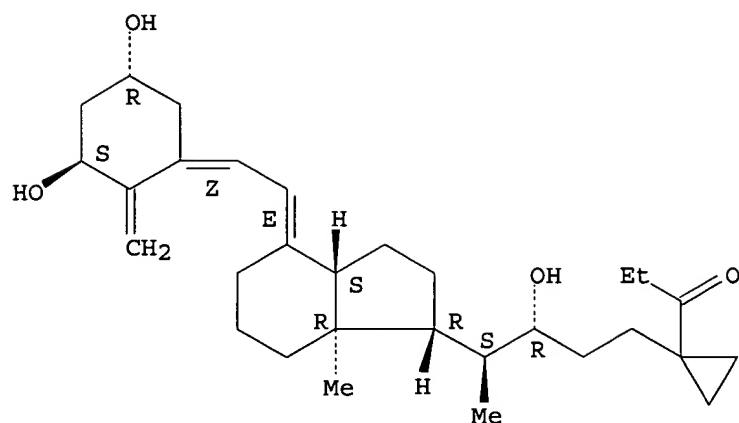
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-37-0 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

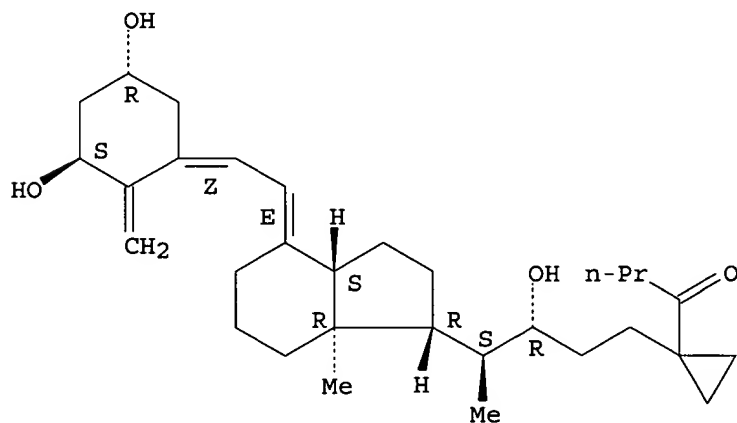
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-44-9 HCAPLUS

CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

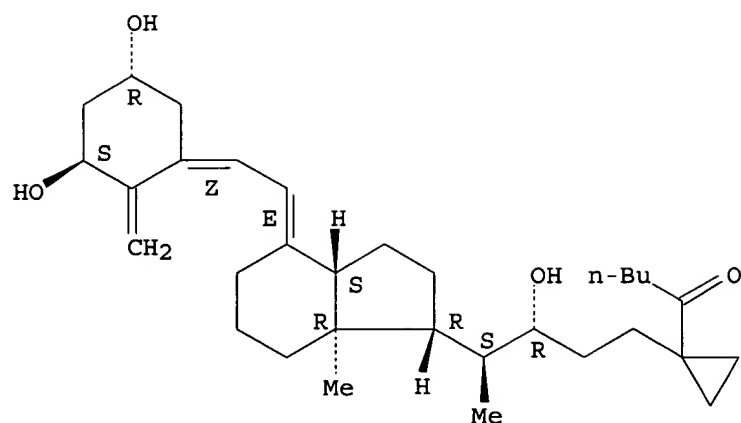
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-54-1 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

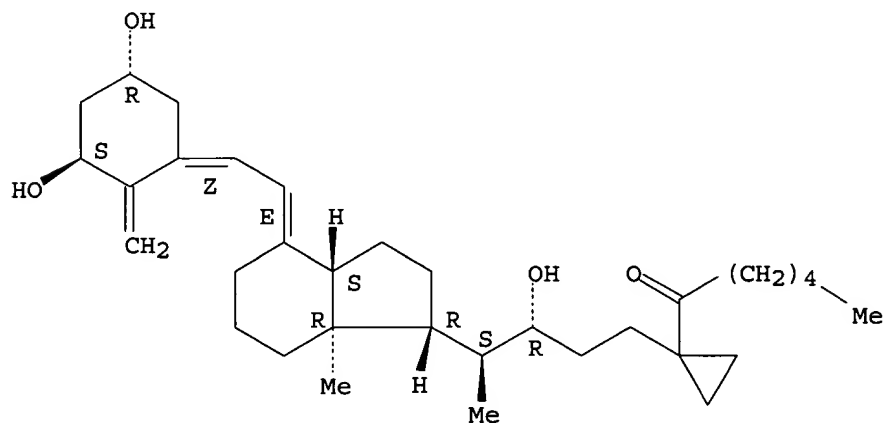
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-64-3 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

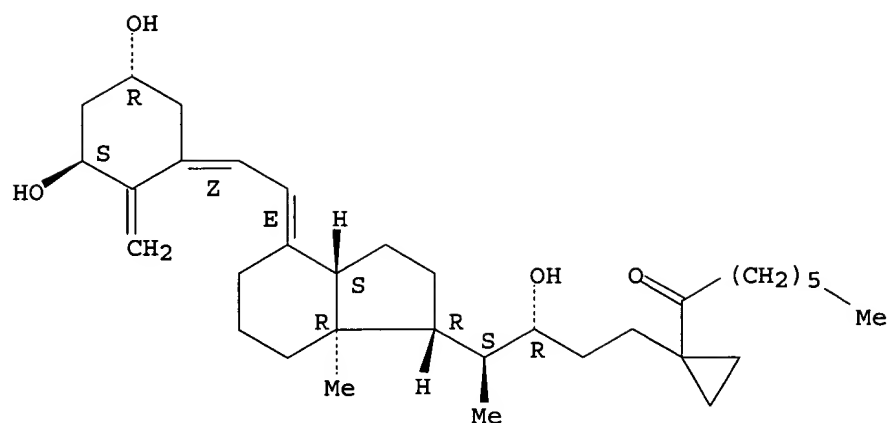
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-80-3 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

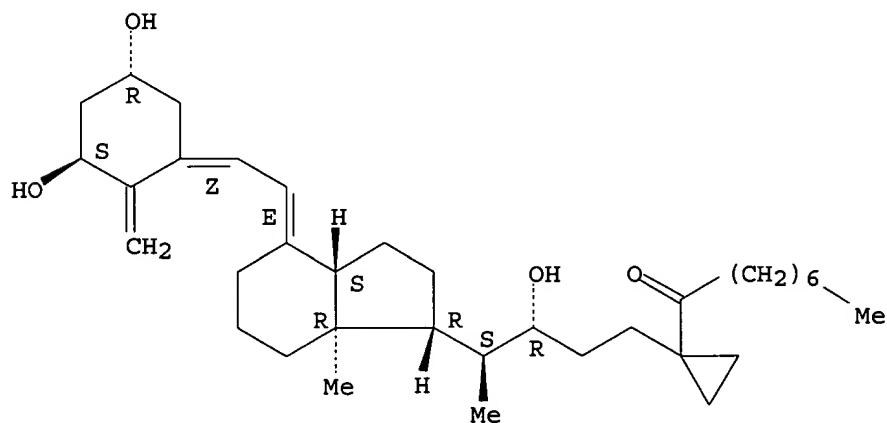
Absolute stereochemistry.
Double bond geometry as shown.



RN 223110-95-0 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

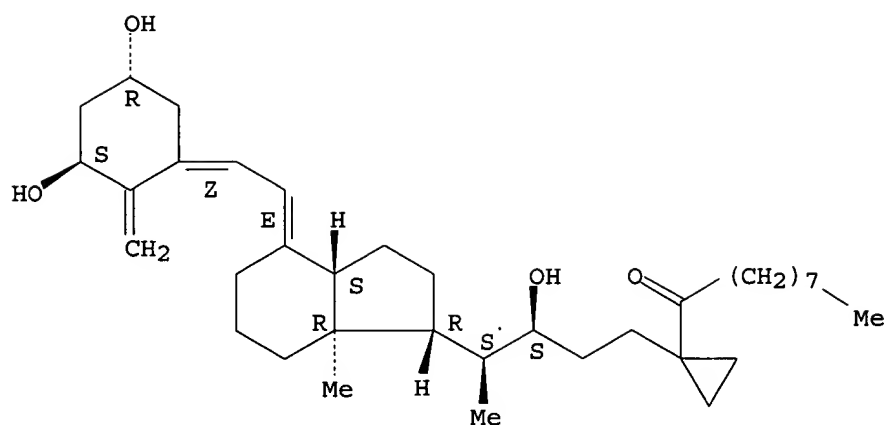
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-01-1 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

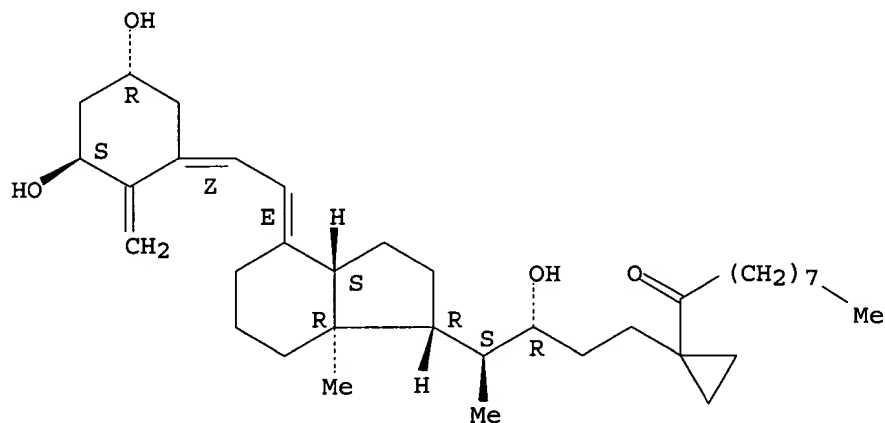
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-11-3 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

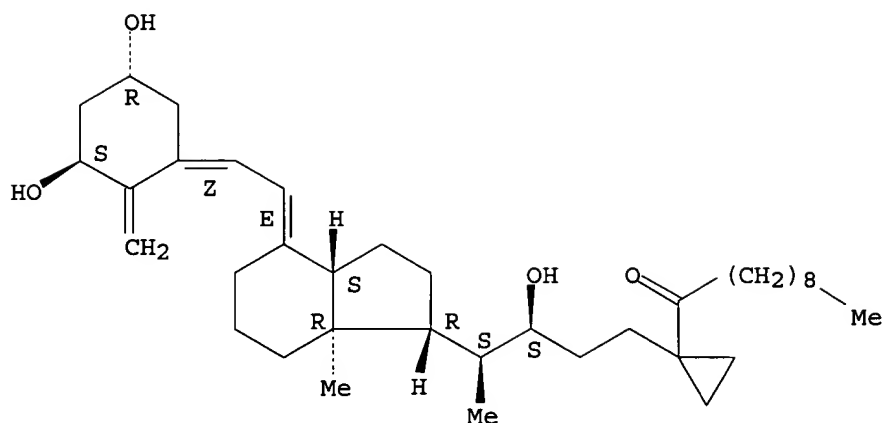
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-22-6 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

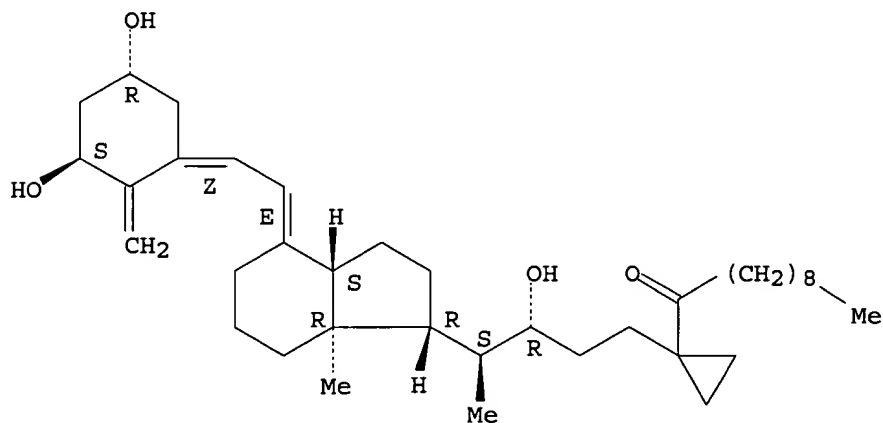
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-31-7 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

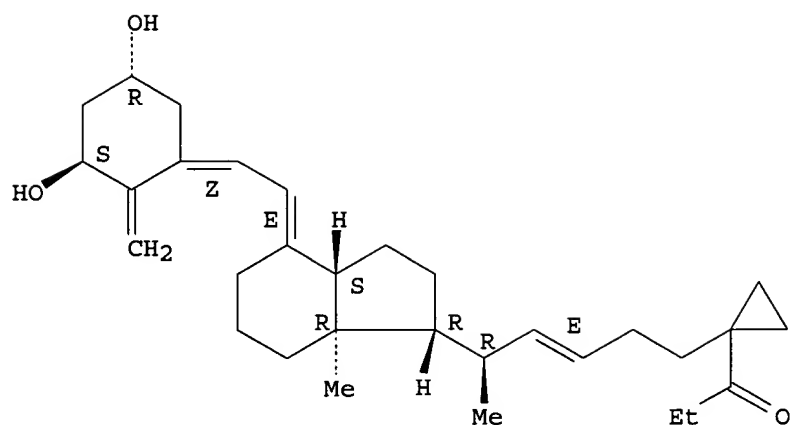
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-41-9 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

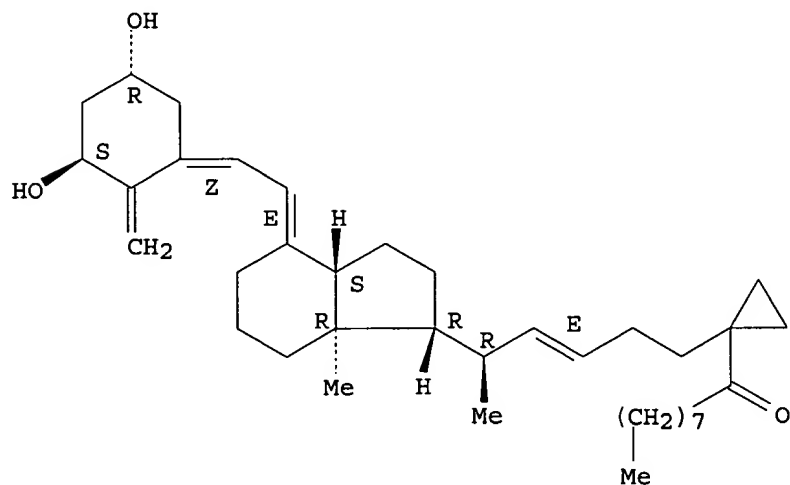
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-46-4 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

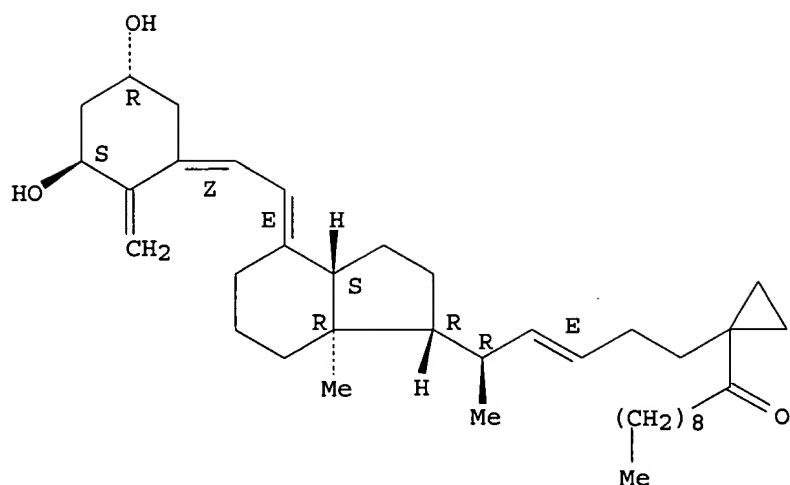
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-53-3 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E)-1,3-dihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19),22-tetraen-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

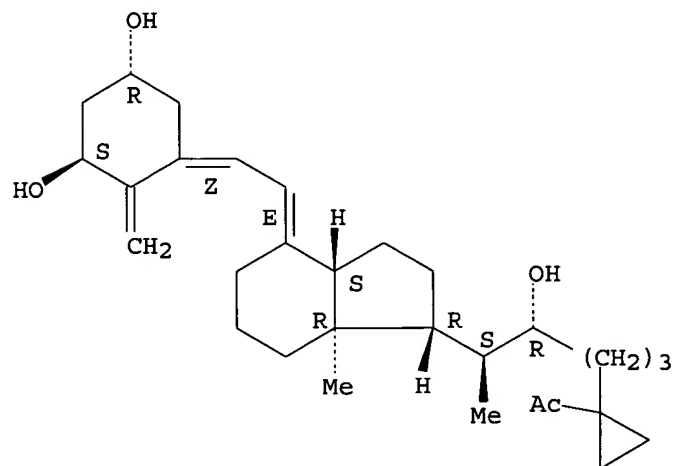
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-57-7 HCAPLUS

CN Ethanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

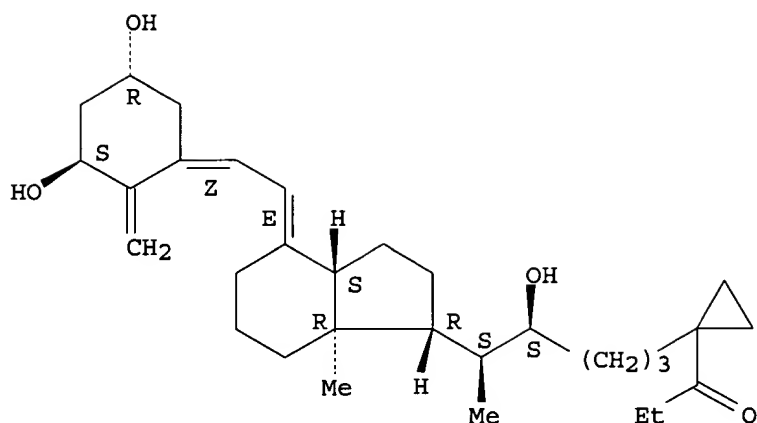
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-62-4 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

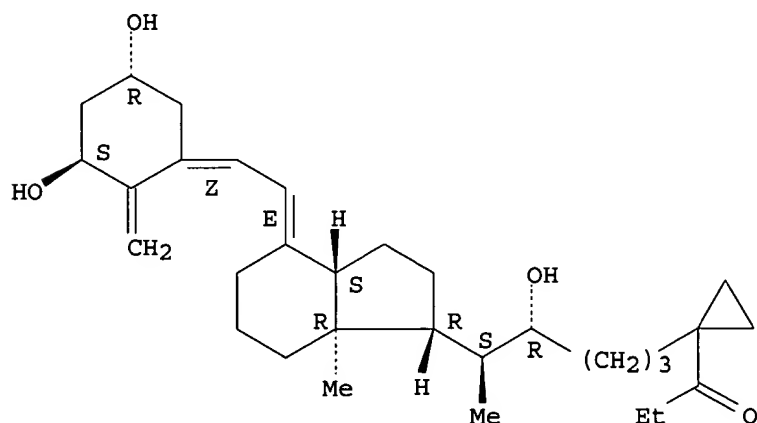
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-67-9 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

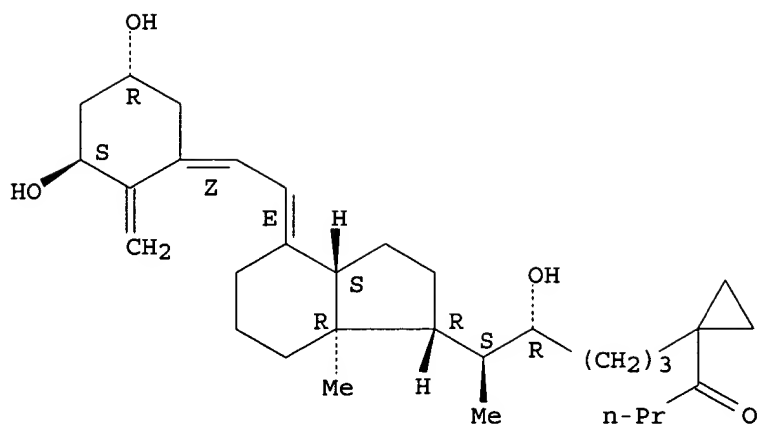
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-73-7 HCAPLUS

CN 1-Butanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

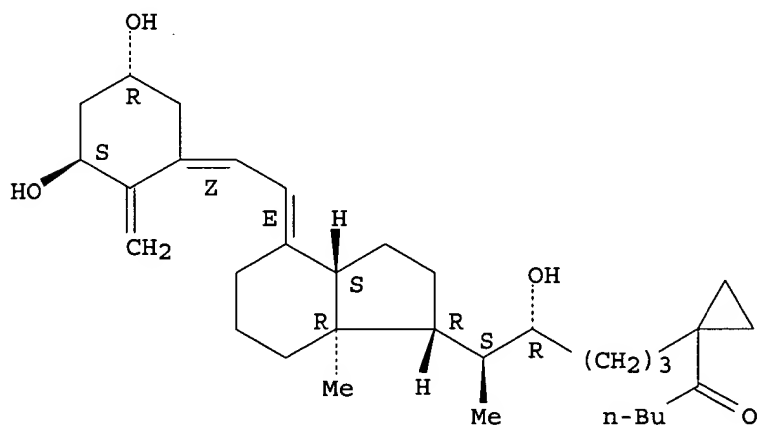
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-80-6 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

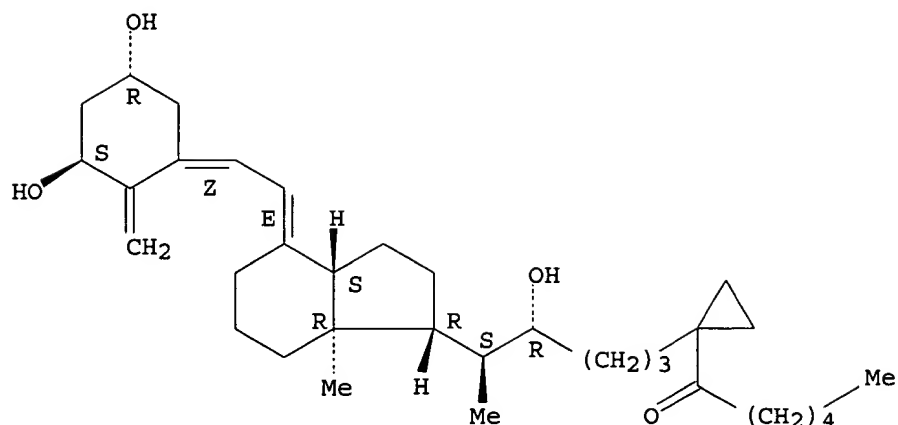
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-86-2 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

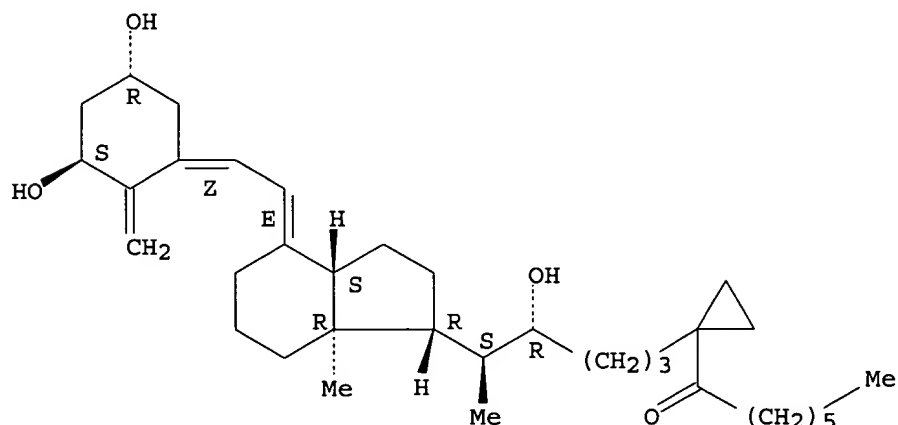
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-89-5 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

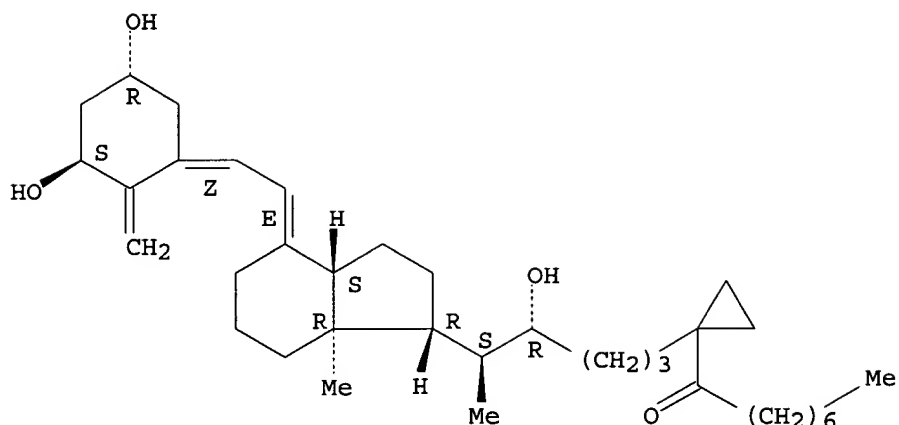
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-94-2 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

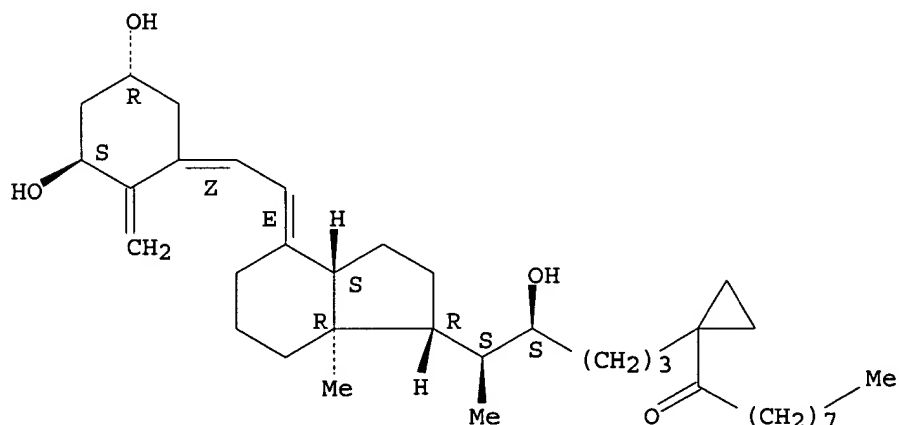
Absolute stereochemistry.
Double bond geometry as shown.



RN 223111-97-5 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

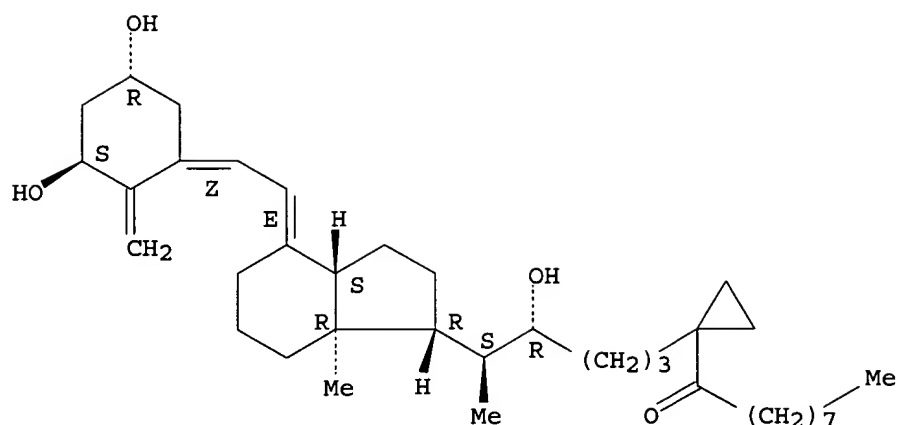
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-01-4 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

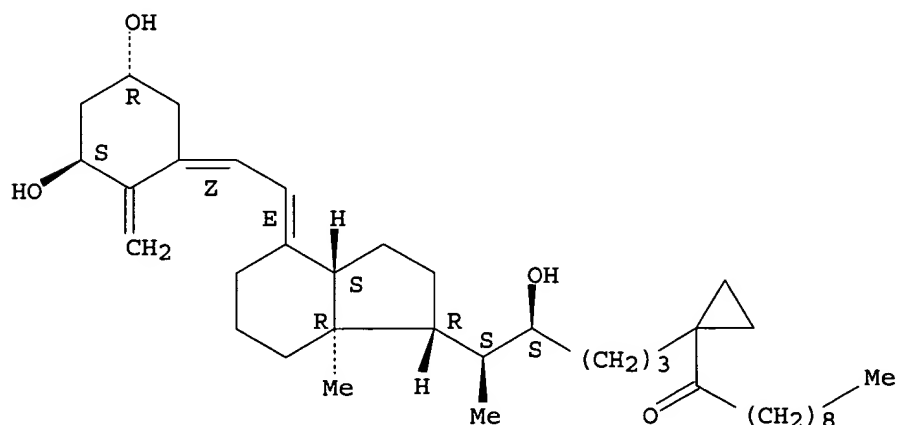
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-04-7 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

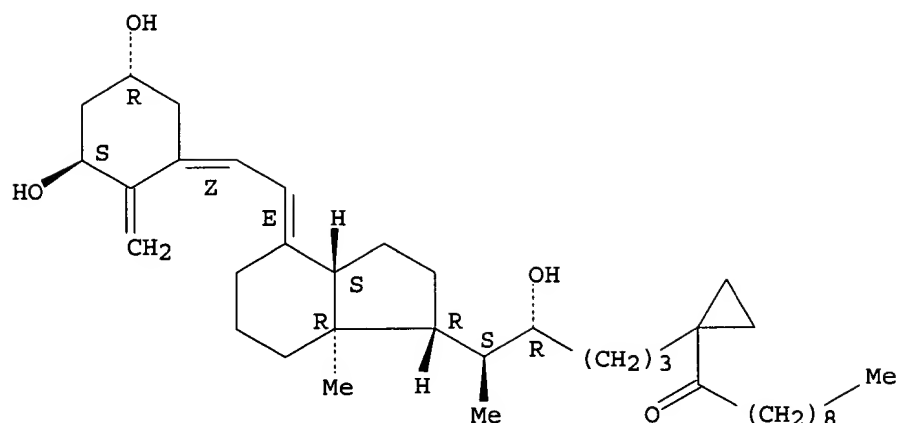
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-06-9 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22R)-1,3,22-trihydroxy-26,27-dinor-9,10-secocholesta-5,7,10(19)-trien-25-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

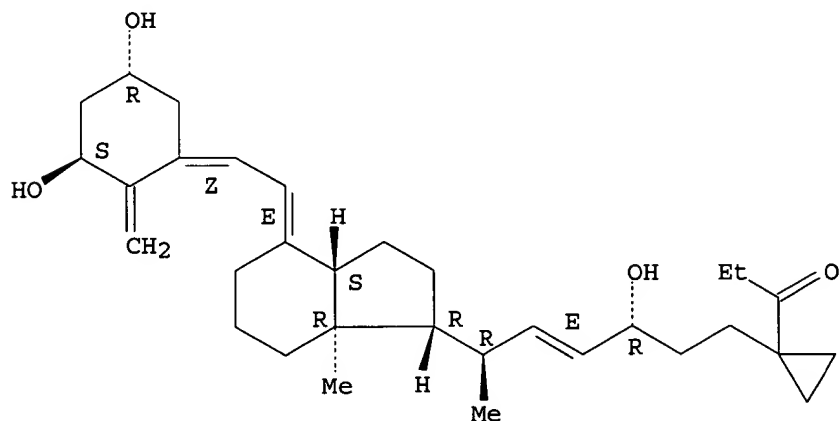
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-10-5 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

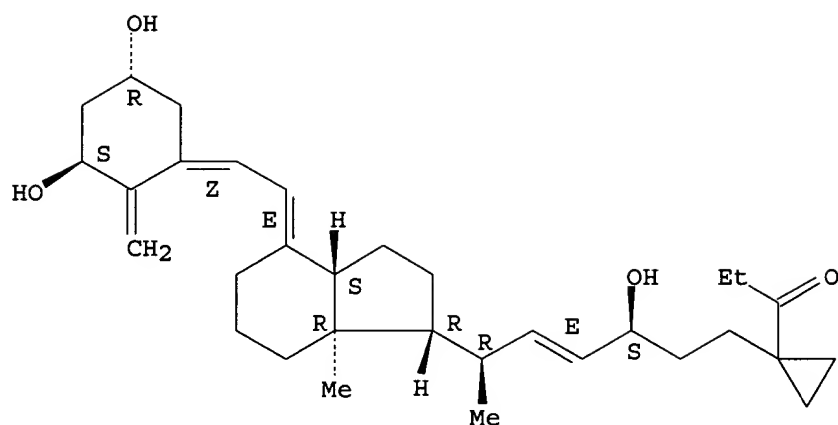
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-13-8 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

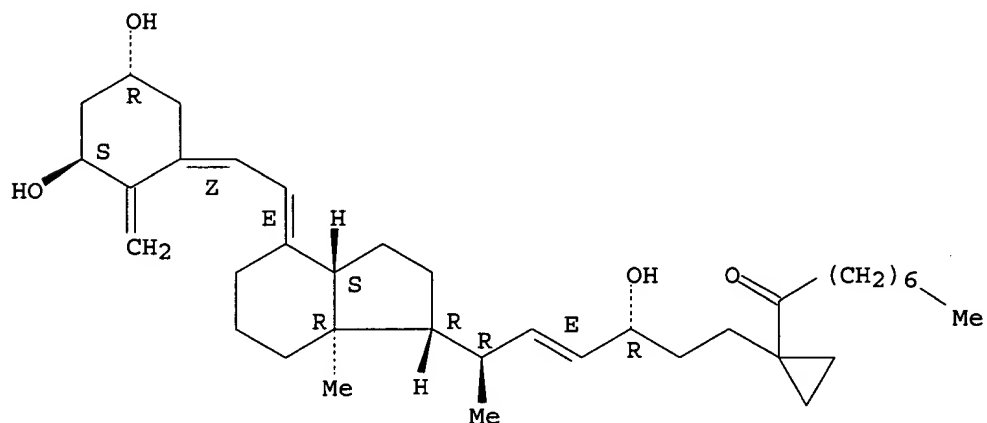
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-15-0 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

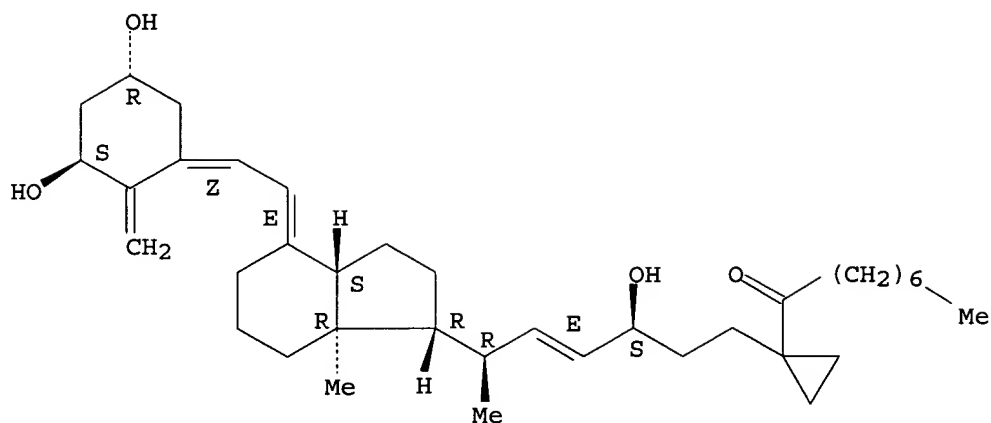
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-17-2 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

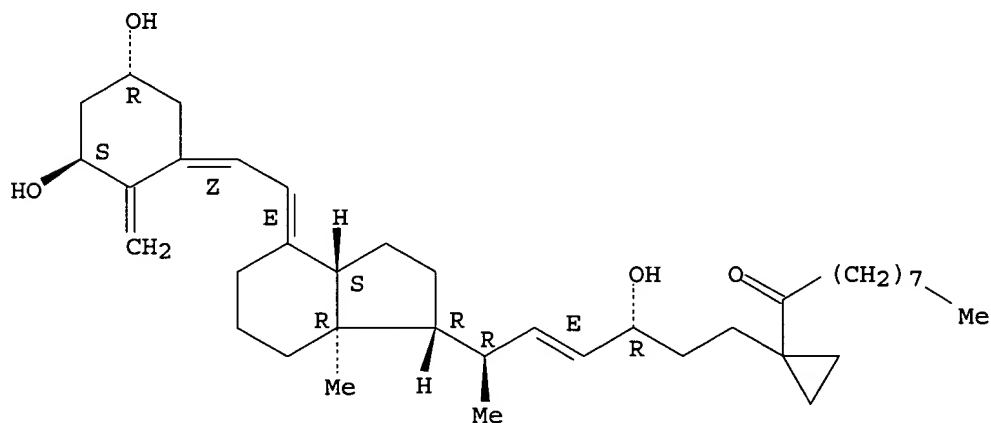
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-18-3 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

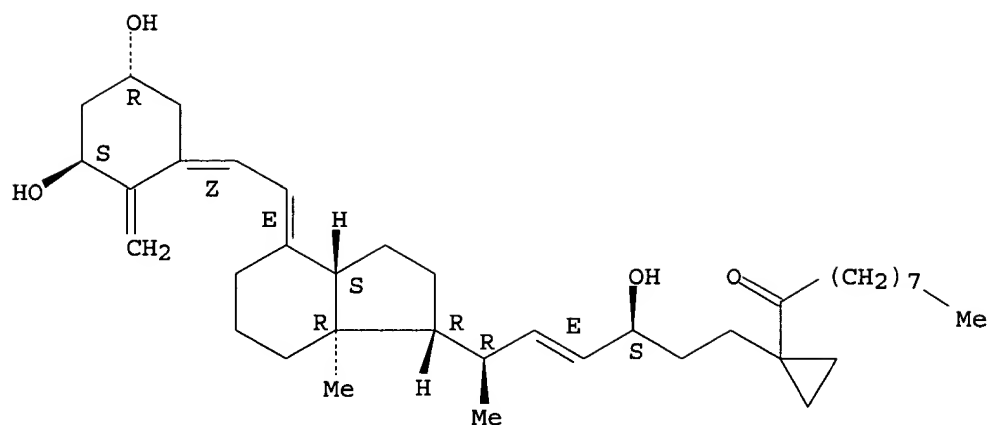
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-19-4 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

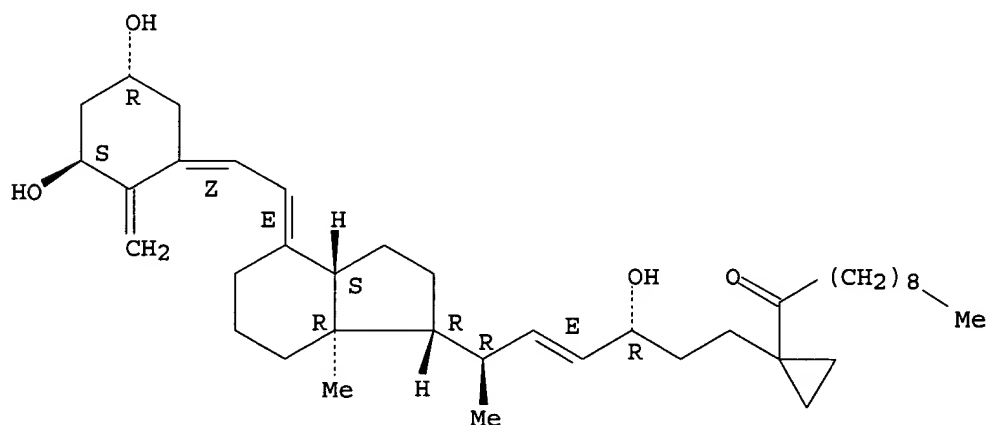
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-20-7 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

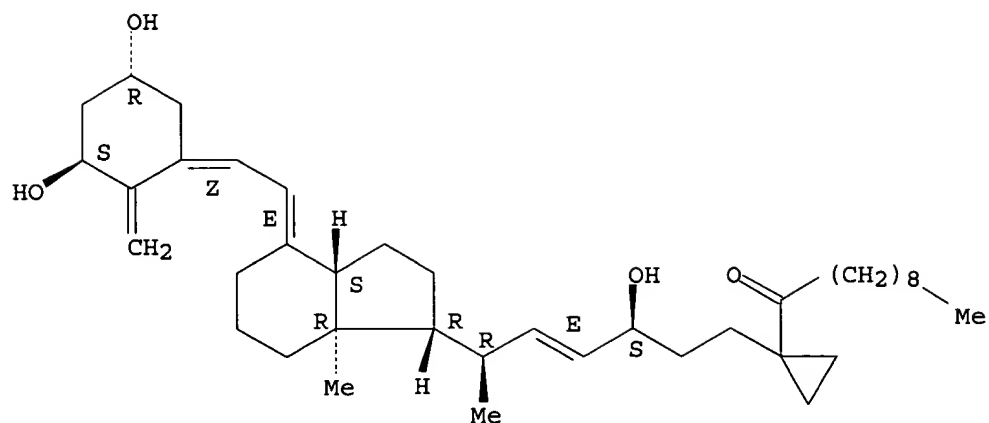
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-21-8 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3,24-trihydroxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

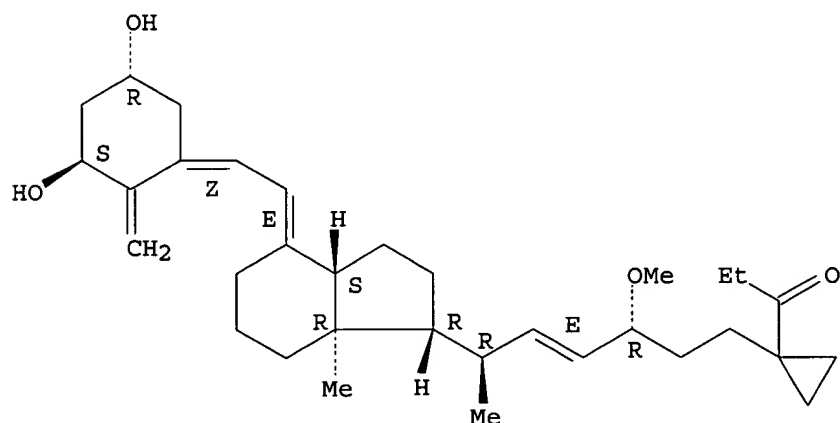
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-23-0 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

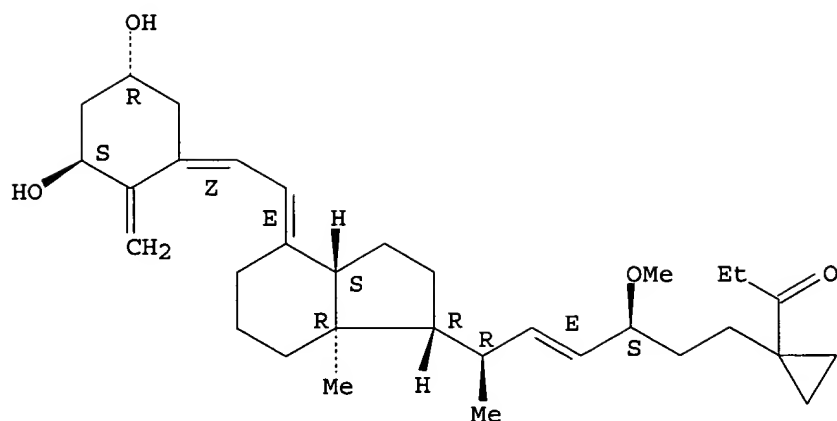
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-25-2 HCAPLUS

CN 1-Propanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

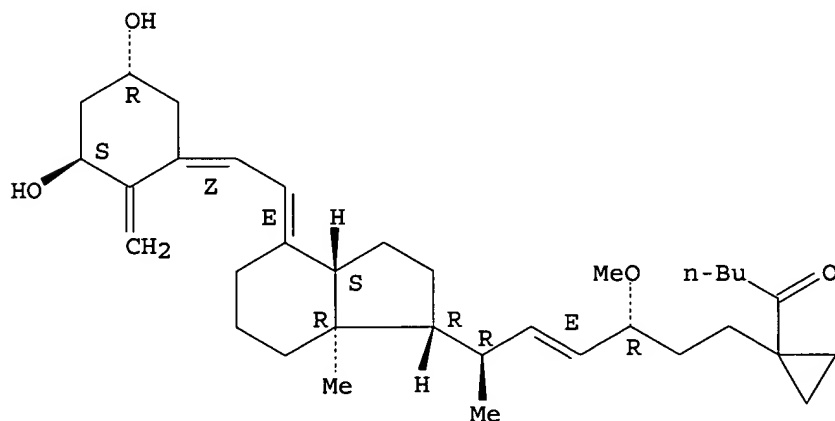
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-27-4 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]-(9CI) (CA INDEX NAME)

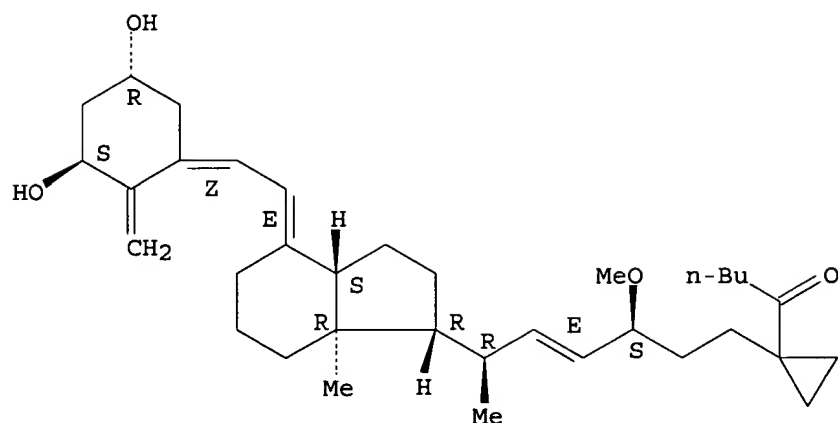
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-28-5 HCAPLUS

CN 1-Pentanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]-(9CI) (CA INDEX NAME)

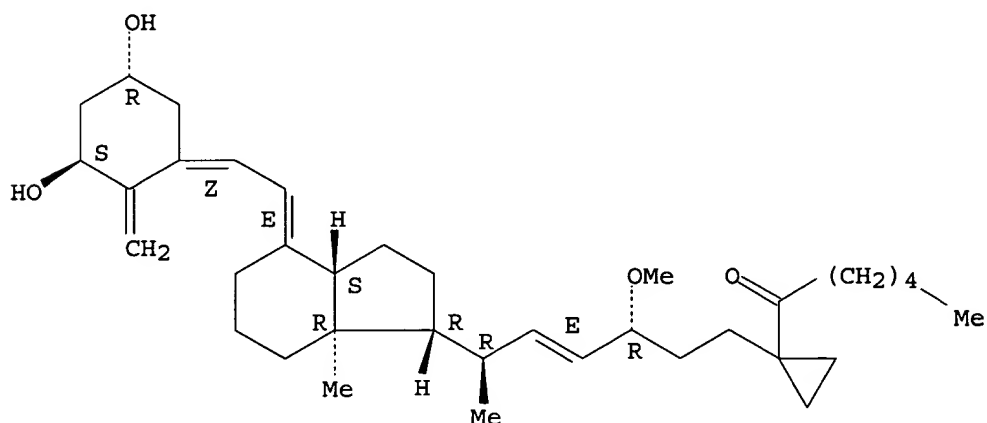
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-31-0 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

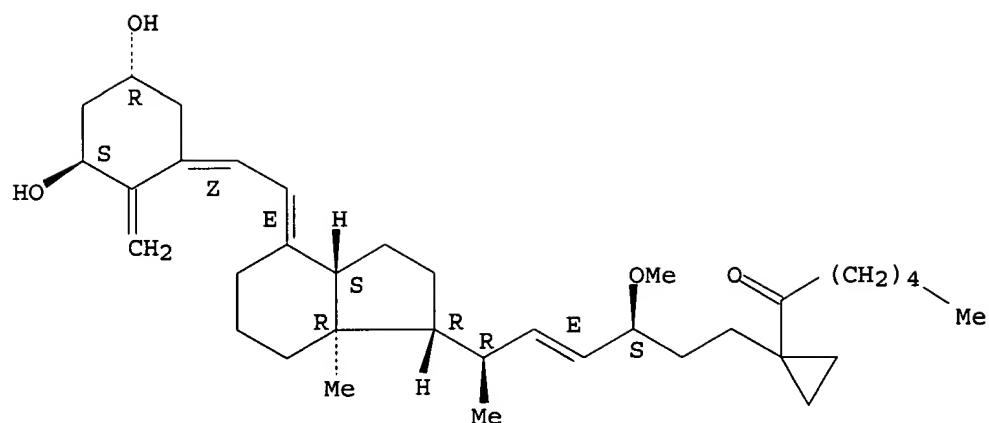
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-35-4 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

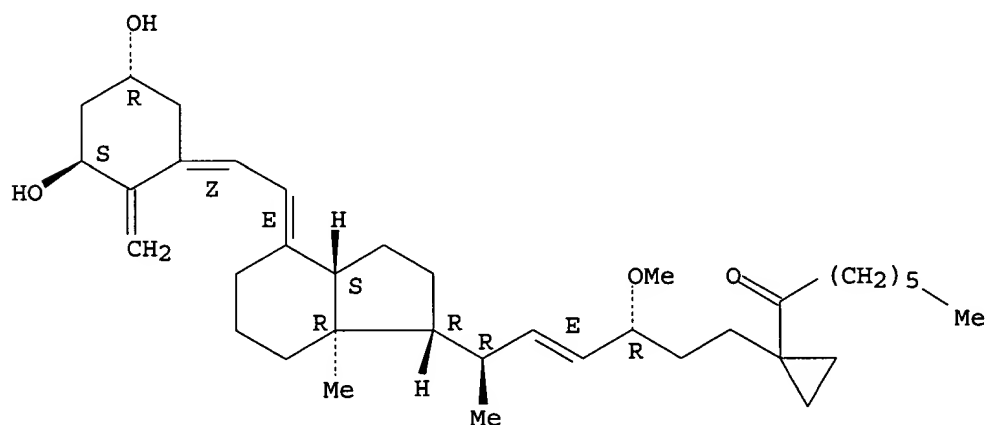
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-39-8 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

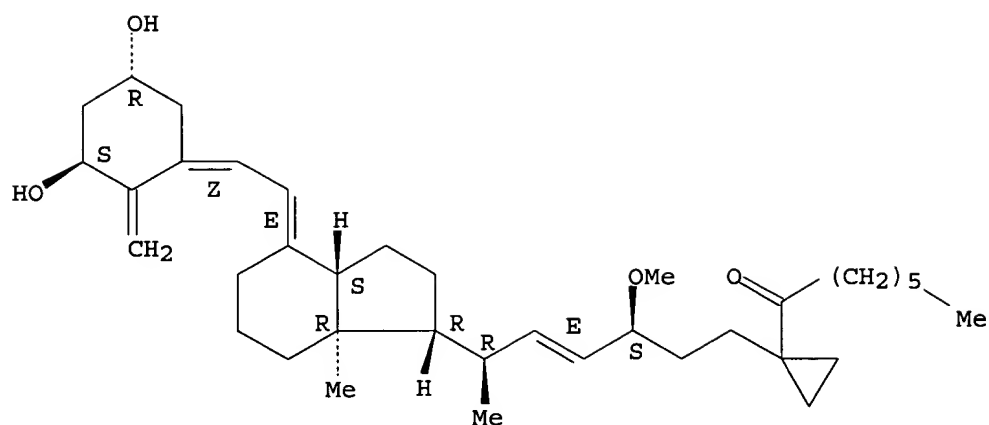
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-43-4 HCAPLUS

CN 1-Heptanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

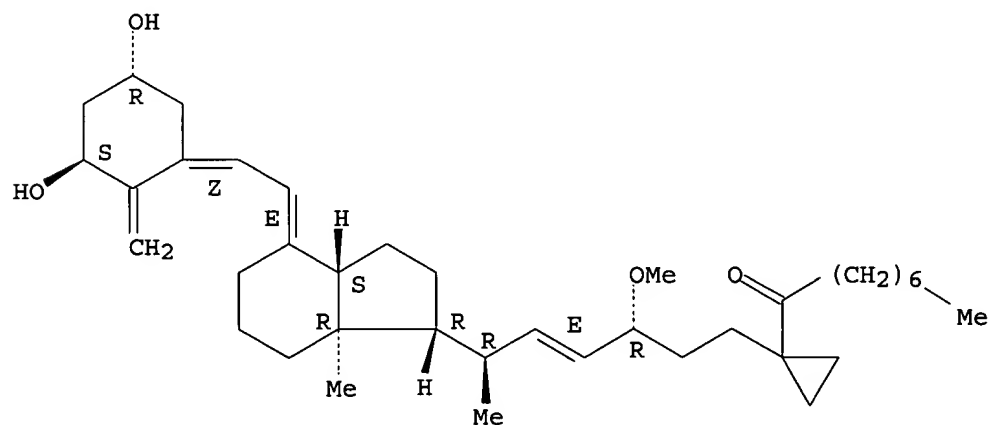
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-48-9 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

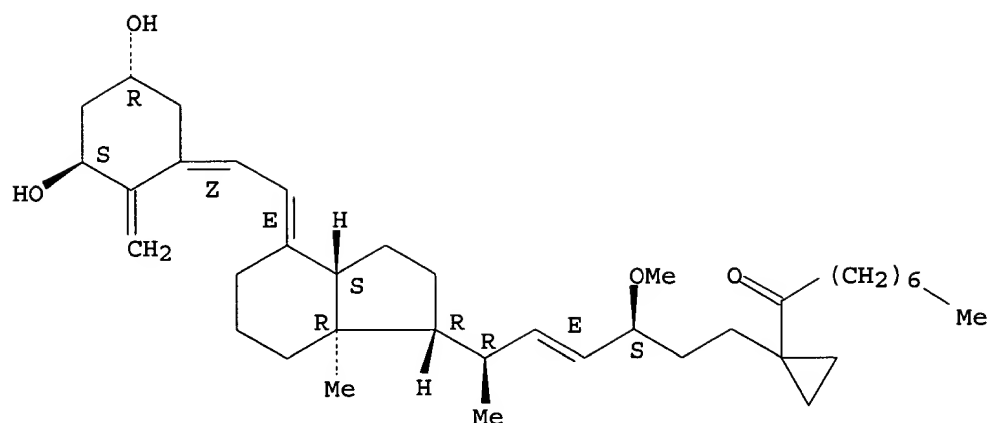
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-52-5 HCAPLUS

CN 1-Octanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

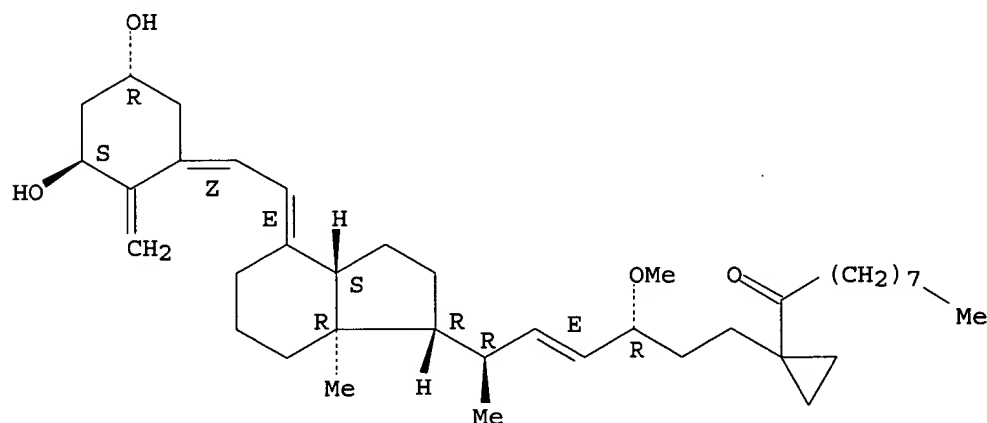
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-54-7 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]-(9CI) (CA INDEX NAME)

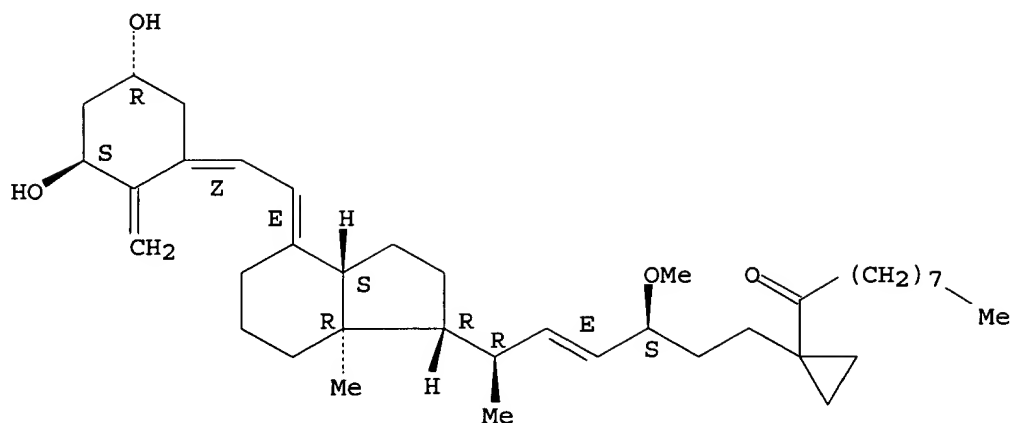
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-57-0 HCAPLUS

CN 1-Nonanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]-(9CI) (CA INDEX NAME)

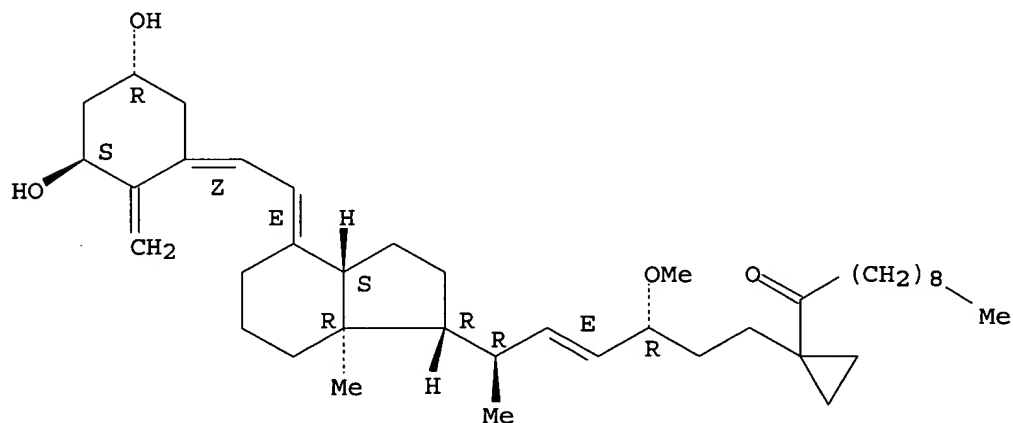
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-60-5 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]-(9CI) (CA INDEX NAME)

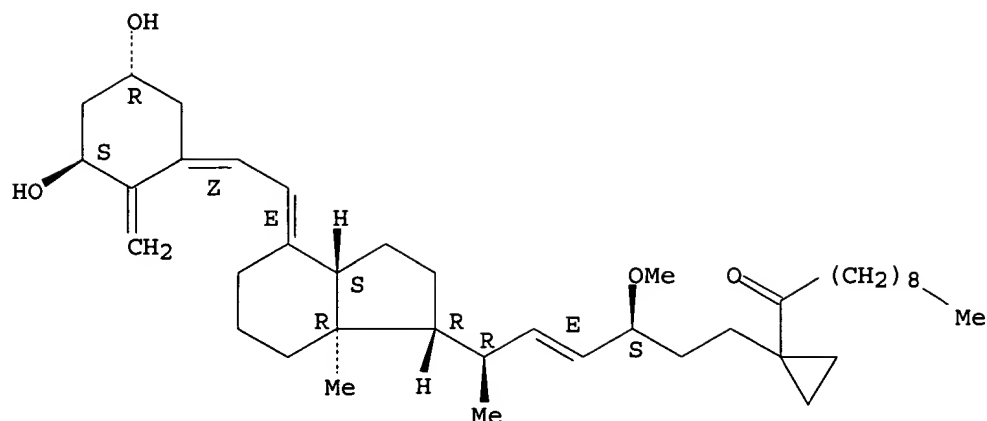
Absolute stereochemistry.
Double bond geometry as shown.



RN 223112-63-8 HCAPLUS

CN 1-Decanone, 1-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-27-nor-9,10-secocholesta-5,7,10(19),22-tetraen-26-yl]cyclopropyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



IT 223107-26-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

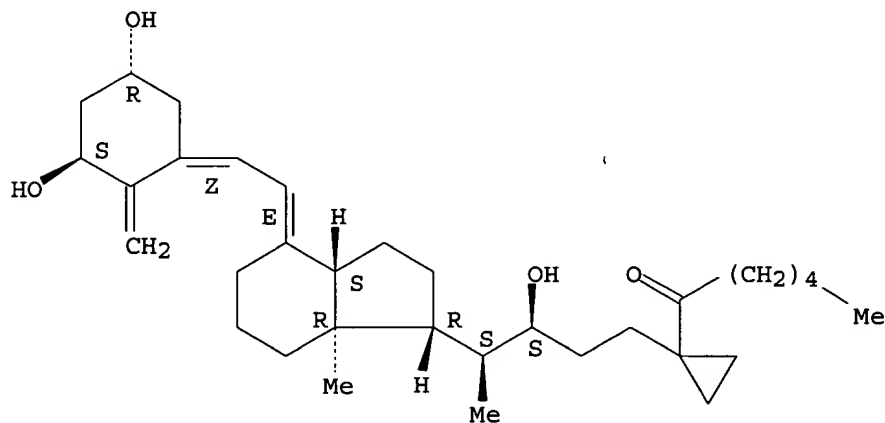
(preparation of novel vitamin D derivs. with cyclopropyl ring in lateral chains and pharmaceutical uses)

RN 223107-26-4 HCAPLUS

CN 1-Hexanone, 1-[1-[(1 α ,3 β ,5Z,7E,22S)-1,3,22-trihydroxy-9,10-secochola-5,7,10(19)-trien-24-yl]cyclopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L53 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:121454 HCAPLUS

DN 126:131696

ED Entered STN: 22 Feb 1997

TI Novel vitamin D derivatives with C-25 substituents for use as antiproliferative agents

IN Kirsch, Gerald; Steinmeyer, Andreas; Neef, Guenter; Schwarz, Katica; Thieroff-Ekerdt, Ruth; Wiesinger, Herbert; Menrad, Andreas; Haberey, Martin

PA Schering A.-G., Germany

SO PCT Int. Appl., 114 pp.

CODEN: PIXXD2

DT Patent

LA German

IC ICM C07C401-00

ICS A61K031-59
CC 32-7 (Steroids)
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9700242	A1	19970103	WO 1996-EP1788	19960430 <--
	W: AU, CA, CN, CZ, FI, HU, JP, KR, MX, NO, NZ, PL, RU, SK, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	CA 2224440	AA	19970103	CA 1996-2224440	19960430 <--
	AU 9656930	A1	19970115	AU 1996-56930	19960430 <--
	AU 707942	B2	19990722		
	EP 832063	A1	19980401	EP 1996-915001	19960430 <--
	EP 832063	B1	20000223		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 11507649	T2	19990706	JP 1996-502535	19960430 <--
	AT 189888	E	20000315	AT 1996-915001	19960430 <--
	ES 2144239	T3	20000601	ES 1996-915001	19960430 <--
	PT 832063	T	20000630	PT 1996-915001	19960430 <--
	CZ 291915	B6	20030618	CZ 1997-4031	19960430 <--
	ZA 9605098	A	19970122	ZA 1996-5098	19960614 <--
	NO 9705852	A	19980216	NO 1997-5852	19971212 <--
	US 6372731	B1	20020416	US 1998-981819	19980331 <--
	GR 3033459	T3	20000929	GR 2000-401148	20000519 <--
	US 6376480	B1	20020423	US 2000-738286	20001218 <--
PRAI	DE 1995-19522797	A	19950614	<--	
	WO 1996-EP1788	W	19960430	<--	
	US 1998-981819	A1	19980331	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9700242	ICM	C07C401-00
	ICS	A61K031-59
WO 9700242	ECLA	C07C401/00
US 6372731	ECLA	C07C401/00
US 6376480	ECLA	C07C401/00

OS MARPAT 126:131696

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Vitamin D derivs. I [Y1 = OH, acyloxy; Y2 = H, Acyl; R1R2 = H2, CH2; R3, R4 = H, Cl, F, alkyl; R3R4 = CH2, alkylene; AB = O; A = OH, acyloxy, B = H; A = H, B = OH, acyloxy; R5, R6 = H, Cl, F, CF3, alkyl; R5R6 = (un)substituted alkylene] were prepared Thus, I [Y1 = OH, Y2 = H, R1R2 = CH2, R3 = H, R4 = Me, A = OH, B = H, R5R6 = CH2CH2, Z = Ac] was obtained from the acid II in 4 steps. This compound had twice the cell differentiating activity of calcitriol.

ST vitamin D deriv prepn antiproliferative; calcitriol antagonist vitamin D deriv prepn; receptor affinity vitamin D deriv

IT Antitumor agents
(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

IT Vitamin D receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(receptor affinity of 25-substituted vitamin D derivs.)

IT 32222-06-3, Calcitriol
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(antagonists; preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

IT 186371-79-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

IT 186371-78-8P 186371-80-2P 186371-81-3P 186371-82-4P 186371-84-6P
186371-87-9P 186371-90-4P 186371-91-5P 186371-96-0P 186372-00-9P
186372-11-2P 186372-12-3P 186372-14-5P 186372-15-6P 186372-27-0P
186372-29-2P 186372-42-9P 186372-48-5P 186372-53-2P 186372-57-6P
186372-79-2P 186372-80-5P 186372-88-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

IT 627-19-0, 1-Pentyne 867-13-0, Triethyl phosphonoacetate 38806-09-6
66703-03-5, (E)-1-Iodo-1-pentene 112828-12-3 112828-13-4 139356-39-1
156965-22-9 163208-17-1 186371-85-7 186371-98-2 186372-01-0
186372-30-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

IT 112924-91-1P 112924-92-2P 124572-91-4P 124572-92-5P 124573-09-7P
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186371-86-8P 186371-92-6P 186371-93-7P 186371-94-8P 186371-95-9P
186371-99-3P 186372-06-5P 186372-07-6P 186372-09-8P 186372-10-1P
186372-13-4P 186372-16-7P 186372-19-0P 186372-20-3P 186372-23-6P
186372-26-9P 186372-31-6P 186372-32-7P 186372-33-8P 186372-34-9P
186372-35-0P 186372-36-1P 186372-37-2P 186372-38-3P 186372-39-4P
186372-40-7P 186372-44-1P 186372-45-2P 186372-46-3P 186372-49-6P
186372-50-9P 186372-51-0P 186372-54-3P 186372-55-4P 186372-56-5P
186372-59-8P 186372-60-1P 186372-61-2P 186372-64-5P 186372-65-6P
186372-66-7P 186372-69-0P 186372-70-3P 186372-71-4P 186372-72-5P
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186372-78-1P 186372-81-6P 186372-82-7P 186372-85-0P 186372-86-1P
186372-89-4P 186372-90-7P 186372-94-1P 186372-96-3P 186372-99-6P
186373-00-2P 186373-02-4P 186373-03-5P 186373-04-6P 186373-05-7P
186373-08-0P 186373-09-1P 186373-10-4P 186373-11-5P 186373-13-7P
186373-18-2P 186373-19-3P 186373-20-6P 186373-22-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

IT 186371-77-7P 186371-83-5P 186371-88-0P 186371-89-1P 186371-97-1P
186372-02-1P 186372-03-2P 186372-04-3P 186372-05-4P 186372-17-8P
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 186374-14-1P 186374-15-2P **186374-16-3P 186374-17-4P**
 186374-18-5P 186374-19-6P 186374-20-9P 186374-21-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

IT **186373-06-8P 186373-07-9P 186374-00-5P**
186374-01-6P 186374-16-3P 186374-17-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

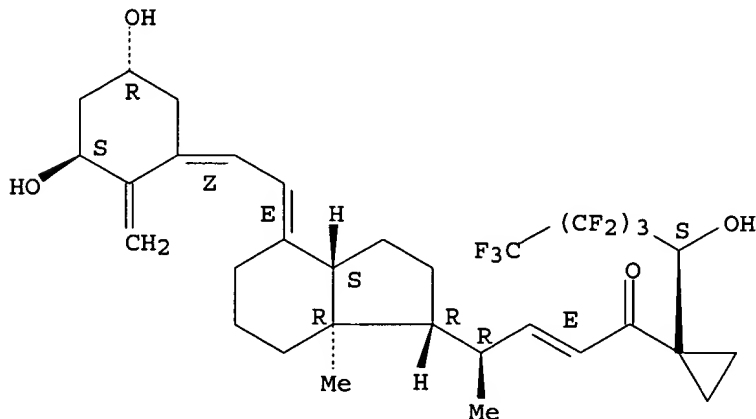
(preparation of 25-substituted vitamin D derivs. with antiproliferative activity)

RN 186373-06-8 HCAPLUS

CN 9,10-Secochole-5,7,10(19),22-tetraen-24-one, 1,3-dihydroxy-24-[1-(2,2,3,3,4,4,5,5,5-nonafluoro-1-hydroxypentyl)cyclopropyl]-, [1 α ,3 β ,5Z,7E,22E,24(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

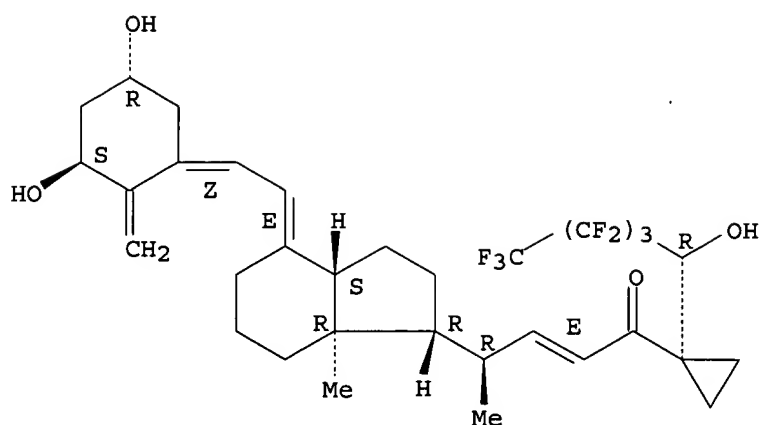


RN 186373-07-9 HCAPLUS

CN 9,10-Secochole-5,7,10(19),22-tetraen-24-one, 1,3-dihydroxy-24-[1-(2,2,3,3,4,4,5,5,5-nonafluoro-1-hydroxypentyl)cyclopropyl]-, [1 α ,3 β ,5Z,7E,22E,24(R)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

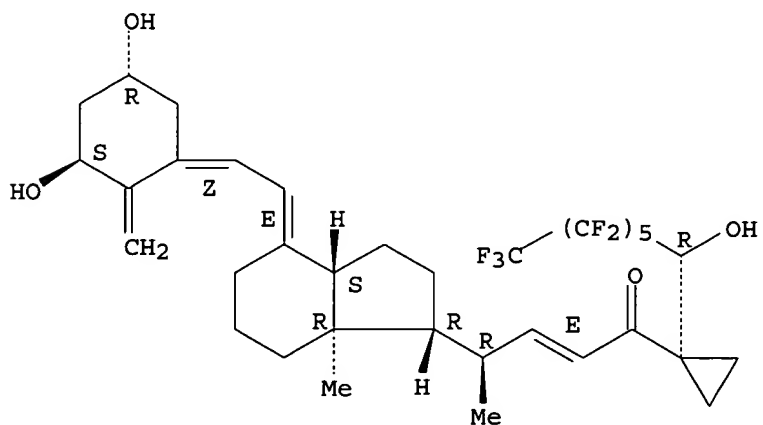
Double bond geometry as shown.



RN 186374-00-5 HCAPLUS

CN 9,10-Secochola-5,7,10(19),22-tetraen-24-one, 1,3-dihydroxy-24-[1-(2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoro-1-hydroxyheptyl)cyclopropyl]-, [1 α ,3 β ,5Z,7E,22E,24(R)]- (9CI) (CA INDEX NAME)

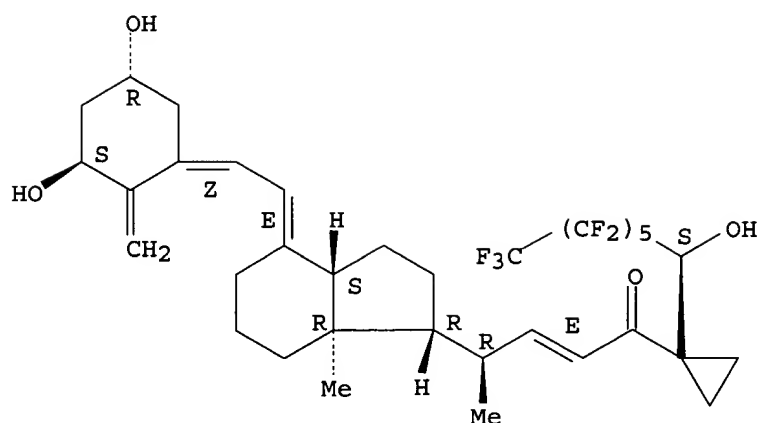
Absolute stereochemistry.
Double bond geometry as shown.



RN 186374-01-6 HCAPLUS

CN 9,10-Secochola-5,7,10(19),22-tetraen-24-one, 1,3-dihydroxy-24-[1-(2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoro-1-hydroxyheptyl)cyclopropyl]-, [1 α ,3 β ,5Z,7E,22E,24(S)]- (9CI) (CA INDEX NAME)

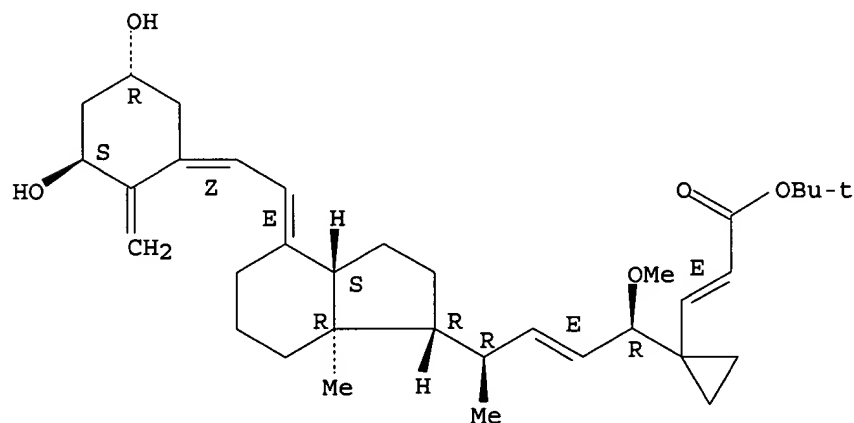
Absolute stereochemistry.
Double bond geometry as shown.



RN 186374-16-3 HCAPLUS

CN 2-Propenoic acid, 3-[1-[(1 α ,3 β ,5Z,7E,22E,24R)-1,3-dihydroxy-24-methoxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]-, 1,1-dimethylethyl ester, (2E)-(9CI) (CA INDEX NAME)

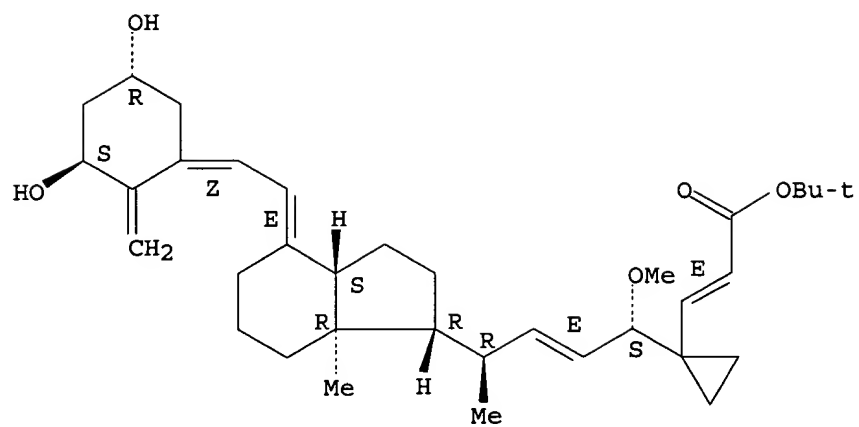
Absolute stereochemistry.
Double bond geometry as shown.



RN 186374-17-4 HCAPLUS

CN 2-Propenoic acid, 3-[1-[(1 α ,3 β ,5Z,7E,22E,24S)-1,3-dihydroxy-24-methoxy-9,10-secochola-5,7,10(19),22-tetraen-24-yl]cyclopropyl]-, 1,1-dimethylethyl ester, (2E)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



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